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A compilation of global bio-optical in situ data for ocean-colour satellite applications

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Abstract. A compiled set of in situ data is important to evaluate the quality of ocean-colour satellite data records. Here we describe the data compiled for the validation of the ocean-colour products from the ESA Ocean Colour Climate Change Initiative (OC-CCI). The data were acquired from several sources (MOBY, BOUSSOLE, AERONET-OC, SeaBASS, NOMAD, MERMAID, AMT, ICES, HOT, GEPCO), spans between 1997 and 2012, and have a global distribution. Observations of the following variables were compiled: spectral remote-sensing reflectances, concentrations of chlorophyll-a, spectral inherent optical properties and spectral diffuse attenuation coefficients. The data were from multi-project archives acquired via the open internet services or from individual projects, acquired directly from data providers. Methodologies were implemented for homogenisation, quality control and merging of all data. No changes were made to the original data, other than averaging of observations that were close in time and space, elimination of some points after quality control and conversion to a standard format. The final result is a merged table designed for validation of satellite-derived ocean-colour products and available in text format. Metadata of each in situ measurement (original source, cruise or experiment, principal investigator) were propagated throughout the work and made available in the final table. Using all the data in a validation exercise increases the number of matchups and enhances the representativeness of different marine regimes. By making

available the metadata, it is also possible to analyse each set of data separately. The compiled data are available at http://doi.pangaea.de/10.1594/PANGAEA.854832.

1 Introduction

Currently, there are several bio-optical in situ data sets worldwide suitable for validation of ocean-colour satellite data. While some are managed by the data producers, others are in international repositories with contributions from multiple scientists. Many have rigid quality controls and are built specifically for ocean colour validation. The use of only any one of these data sets would limit the number of data in validation exercises. It would therefore be useful to acquire and merge all these data sets into a single unified data set to maximize the number of matchups available for validation, their distribution in time and space, and consequently reduce the uncertainties in the validation exercise. However, merging several data sets together can be a complicated task. First it is necessary to acquire and harmonize all data sets into a single standard format. Second, during the merging, the duplicates between data sets have to be identified and removed. Third, the metadata should be propagated throughout the process and made available in the final merged product. Ideally, the compiled data set would be made available as a simple text table, to facilitate ease of access and manipulation. In this work such unification of multiple data sets is presented. This was done for the validation of the ocean-colour products from the ESA Ocean Colour Climate Change Initiative (OC-CCI), but with the intent to serve the broad user community as well.

A merged data set is not without drawbacks: it is likely to be large and so not always easy to manipulate; because the merging is done on pre-existing, processed databases, one does not have full command of the whole processing chain; the data set would be a compilation of observations collected by several investigators using different instruments, sampling methods and protocols, which might eventually have been modified by the processing routines used by the repositories or archives. Nevertheless, to minimise these potential drawbacks, we have, for the most part, incorporated only data sets that have emerged from the long-term efforts of the ocean-colour and biological oceanographic communities to provide scientists with high-quality in situ data, and implemented additional quality checks on the data, to enhance confidence in the quality of the merged product.

In Sect. 2 the methodologies used to harmonize and integrate all data, as well as a description of individual data sets acquired are provided. In Sect. 3 the geographic distribution and other characteristics of the final merged data set are shown. Section 4 provides an overview of the results.

2 Data and methods

2.1 Pre-processing and merging

The compiled global set of bio-optical in situ data described in this work has an emphasis, though not exclusive, on open-ocean data from all geographic regions. It is comprised of the following variables: remote-sensing reflectance ("rrs"), chlorophyll-a concentration ("chla"), algal pigment absorption coefficient ("aph"), detrital and coloured dissolved organic matter absorption coefficient ("adg"), particle backscattering coefficient ("bbp") and diffuse attenuation coefficient for downward irradiance ("kd"). A similar effort of compiling bio-optical in situ data from different sources has been recently published by Nechad et al. (2015). Given their focus on selected coastal regions, most of the data presented here is not part of their compilation. The variables "rrs", "aph", "adg", "bbp" and "kd" are spectrally dependent, and this dependence is hereafter implied. The data were compiled from 10 sources of in situ data (MOBY, BOUSSOLE, AERONET-OC, SeaBASS, NOMAD, MERMAID, AMT, ICES, HOT, GEPCO) each one described in Sect. 2.2. The compiled in situ observations have a global distribution and cover the recent period of satellite ocean-colour data between 1997 and 2012. The listed variables were chosen as they are the operational satellite ocean-colour products of ESA OC-CCI project, which currently focuses on the use of three ocean-colour satellite platforms: the Medium Resolution Imaging Spectrometer (MERIS) of ESA; the Moderate Resolution Imaging Spectro-radiometer (MODIS) of NASA; and the Sea-viewing Wide Field-of-view Sensor (SeaWiFS) of NASA, to create a time series of satellite data.

Remote-sensing reflectance ("rrs") is a primary ocean colour product routinely produced by several space agencies. It is defined as “rrs = Lw/Es”, where “Lw” is the upward water-leaving radiance and “Es” is the total downward irradiance at sea level. Remote-sensing reflectance is related to irradiance reflectance (“Rw”) approximately through “rrs = Rw/Q”, where Q ranges from 3 to 5 in natural waters and is equal to π for an isotropic (Lambertian) light field. Another quantity that is often required is the “normalized” water-leaving radiance (“nLw”) (Gordon and Clark, 1981), which is related to remote-sensing reflectance via “rrs = nLw/Fo”, where "Fo" is the top-of-the-atmosphere solar irradiance. If not directly available, remote-sensing reflectance was calculated through the equations described above, depending on the format of the original data. The original data were acquired in an advanced form (e.g. time-averaged, extrapolated to surface), from 6 data sources particularly designed for ocean-colour validation (MOBY, BOUSSOLE, AERONET-OC, SeaBASS, NOMAD, MERMAID), therefore only requiring the conversion to a common format. In the processing made by the space agencies, the quantity “rrs” is normalized to a single Sun-viewing geometry (Sun at zenith and nadir viewing) taking in account the bidirectional effects as described in Morel and Gentili (1996) and Morel et al. (2002). Thus, for consistency with satellite “rrs” product, only in situ “rrs” that included the latter normalization were included in the compilation.

Chlorophyll-a concentration is the traditional measure for phytoplankton biomass and is the most-widely used satellite ocean-colour product. To validate satellite-derived chlorophyll-a concentration, two different variables were compiled: one of these represents chlorophyll-a measurements made through fluorometric or spectrophotometric methods, but for abbreviation it is referred from hereafter as “chla_fluor” and the other is the chlorophyll concentration derived from HPLC measurements, referred-to hereafter as “chla_hplc”. The chlorophyll data were compiled from 8 data sources: BOUSSOLE, SeaBASS, NOMAD, MERMAID, AMT, ICES, HOT, GEPCO. One requirement for “chla_fluor” measurements was that they were made using in vitro methods (i.e. based on extractions of chlorophyll-a). Although this severely decreased the number of observations, since in situ fluorometry (e.g. fluorometers mounted on CTD's) is widely available in oceanographic databases, it was decided to exclude such data because of potential problems with the calibration of in situ fluorometers. The variable “chla_hplc” was calculated by summing all reported chlorophyll-a derivatives, including divinyl chlorophyll-a, epimers, allomers, and chlorophyllide-a. The two chlorophyll variables are retained separately in the database to facilitate their use. HPLC measurements are considered of higher quality, but fluorometric measurements are more abundant. Thus one option for users is to use “chla_fluor” only when there are no “chla_hplc” measurements available. To be consistent with satellite-derived chlorophyll values, which are derived from the light emerging from the upper layer of the ocean, all chlorophyll observations found in the top 10 meters (replicates at the same depth, or measurements at multiple depths) were averaged if the coefficient of variation among observations was less than 50 %, otherwise they were discarded. The averages were then assigned to the surface. The depth of 10 m was chosen as a compromise between clear oligotrophic and turbid eutrophic waters. Other methods, such as chlorophyll depth-averages using local attenuation conditions (Morel and Maritorena, 2001), require observations at multiple depths, which, given our decision to use only in vitro measurements, would have reduced considerably the final number of observations.

With regard to the inherent optical properties ("aph", "adg", "bbp"), if not already calculated and provided in the contributed data sets, they were computed from related variables that were available: particle absorption ("ap"), detrital absorption ("ad"), "Coloured Dissolved Organic Matter" absorption ("ag"), total backscattering ("bb"). The following equations were used “adg = ad + ag”, “ap = aph + ad”, and “bb = bbp + bbw”. For the latter equation, the variable "bbw" was computed using “bbw = bw/2”, where "bw" is the scattering coefficient of seawater derived from Zhang et al. (2009). The diffuse attenuation coefficient for downward irradiance (“kd”) did not require any conversion and was compiled as originally acquired. Observations of inherent optical properties (surface values) and diffuse attenuation coefficient for downward irradiance, were acquired from 3 data sources particularly designed for ocean-colour validation (SeaBASS, NOMAD, MERMAID), thus already subject of the processing routines of these data sets.

The merged data set was compiled from 10 sets of in situ data, which were obtained individually either from archives that incorporate data from multiple contributors (SeaBASS, NOMAD, MERMAID and ICES) or from particular measurement programs or projects (MOBY, BOUSSOLE, AERONET-OC, HOT, GEPCO, AMT) and were subsequently, homogenized and merged. Data contributors are listed in Table 2 and in the auxiliary material. There were methodological differences between data sets. Therefore, after acquisition, and prior to any merging, each set of data was pre-processed for quality control and conversion to a common format. During this process, data were discarded if they had: 1) unrealistic or missing, date, time, and geographic coordinate fields; 2) poor quality (e.g. original flags) or method of observation that did not meet the criteria for the data set (e.g. in situ fluorescence for chlorophyll concentration); and 3) spuriously high or low data. For the latter, the following limits were imposed: for “chla_fluor” and “chla_hplc” [0.001-100] mg m^{-3}; for “rrs” [0-0.15] sr^{-1}; for “aph”, “adg” and “bbp” [0.0001-10] m^{-1}; for “kd” [(aw(λ)-10] m^{-1}, where “aw” are the pure water absorption coefficients derived from Pope and Fry (1997). Also during this stage, three metadata strings were attributed to each observation:

“dataset”, “subdataset” and “pi”. The “dataset” contains the name of the original set of data, and can only be one of the following: “aoc”, “boussole”, “mermaid”, “moby”, “nomad”, “seabass”, “hot”, “ices”, “amt”, “gepco”. The “subdataset” starts with the “dataset” identifier and is followed by additional information about the data, as <dataset>_<cruise/station/site>) (e.g. “seabass_car71”). The “pi” contains the name of the Principal Investigator(s). An effort was made to homogenize the names of Principal Investigators from the different sets of data. These three metadata are the link to trace each observation to its origin and were propagated throughout the processing. Finally, this processing stage ended with each set of data being scanned for replicate variable data and replicate station data, which when found, were averaged if the coefficient of variation was less than 50 %, otherwise they were discarded. Replicates were defined as multiple observations of the same variable, with the same date, time, latitude, longitude and depth. Replicate station data were defined as multiple measurements of the same variable, with the same date, time, latitude and longitude. For the latter case, a search window of 5 minutes in time and 200 meters in distance was given, to account for station drift. A small number of observations that were identified as replicates had a different “subdataset” identifiers (i.e. different cruise name). These observations were considered suspicious if the values were different, and discarded. If the values were the same, one of the observations was retained. This possibly originated from the same group of data being contributed to an archive by two different Principal Investigators.

Once each set of data was homogenized, all data was integrated into a unique table. This final merging focused on the removal of duplicates between the sets of data. Although some duplicates are known (e.g. MOBY, BOUSSOLE, AERONET-OC and NOMAD data are found in SeaBASS and MERMAID sets of data), others are unknown (e.g. how much of GEPCO, ICES, AMT, HOT is within NOMAD, SeaBASS and MERMAID). Therefore, duplicates were identified using the metadata ("dataset" and "subdataset") when possible, and temporal-spatial matches, as an additional precaution. For temporal-spatial matches, several thresholds were used, but typically 5 minutes and 200 meters were taken to be enough to identify most duplicated data, which reflected small differences in time, latitude and longitude, between the different sets of data. Larger thresholds were used in some cases as a cautionary procedure. This was the case when searching for NOMAD data in other data sets, because NOMAD includes a few cases where merging of radiometric and pigment data was done with large spatial-temporal thresholds (Werdell and Bailey, 2005). In regard to all data, if duplicates were found, data from the NOMAD data set were selected first, followed by data from individual projects (MOBY, BOUSSOLE, AERONET-OC, AMT, HOT and GEPCO) and finally for the remaining data sets (SeaBASS, MERMAID and ICES). This procedure was chosen to preserve the NOMAD data set as a whole, since it is widely used in ocean-colour validation. After all data were free of duplicates, they were merged consecutively by variable in the final table. During this process, we also searched for rows (stations) that were separated from each other by time differences less than 5 minutes and horizontal spatial differences of less than 200 meters. When such rows were found, the observations in those rows were merged into a single row. The compiled merged data were compared with the original sets to certify that no errors occurred during the merging. As a final step, a water-column (station) depth was recorded for each observation, which was the closest water column depth from the

ETOPO1 global relief model (National Geophysical Data Center ETOPO1; Amante and Eakins, 2009). For observations where the closest water depth was above sea level (e.g. data collected very near the coast), it was given the value of zero.

Data processing thus included two major steps: pre-processing and merging. The first step was related to each set of contributing data sets in particular and aimed to identify problems and convert the data of interest to a standard format. The second step dealt with the integration of all data into one unique file and included the elimination of duplicated data between the individual sets of data acquired. In the next subsections a brief overview of each original set of data is provided.

2.2 Pre-processing of each set of data

2.2.1 Marine Optical Buoy (MOBY)

The Marine Optical Buoy (MOBY) is a fixed mooring system operated by the National Oceanic and Atmospheric Administration (NOAA) that provides a continuous time series of water-leaving radiance and surface irradiance in the visible region of the spectra since 1997. The site is located a few kilometres west of the Hawaiian Island of Lanai where the water depth is about 1200 m. Since its deployment, MOBY measurements have been the primary basis for the on-orbit vicarious calibrations of the SeaWiFS and MODIS ocean colour sensors. A full description of the MOBY system and processing is provided in Clark et al. (2003). Data are freely available for scientific use at the MOBY Gold directory. The products of interest are the “Scientific Time Series” files, which refer to MOBY data averaged over sensor-specific wavelengths and particular hours of the day (around 20-23 UTC). For this work, the satellite band-average products for SeaWiFS, MODIS AQUA and MERIS were compiled from the January 2005 reprocessing for the early data, and from the latest reprocessing for data after 2011. The “inband” average subproduct was used, and to maintain the highest quality, only data determined from the upper two arms ("Lw1") and flagged "good" quality were acquired. Data from the MOBY203 deployment was discarded due to the absence of surface irradiance data. The compiled variable was the remote-sensing reflectance, “rrs”, which was computed from the original water-leaving radiance (“Lw”) and surface irradiance (“Es”). The water-leaving radiances were corrected for the bidirectional nature of the light field (Morel and Gentili, 1996; Morel et al., 2002) using the same look-up table and method as that used in the SeaWiFS Data Analysis System (SeaDAS) processing code. As mentioned before, the MOBY data compiled in this work are sensor-specific. Therefore, attention is necessary to use the correct MOBY data when validating a particular sensor. The way MOBY data are stored in the final merged table is consistent with the original wavelengths; however, these wavelengths can differ from what is sometimes expected to be the central wavelength of a given band and sensor. Irrespective of the wavelength where MOBY data are stored in the final table, for validation of bands 1-6 of SeaWiFS, MOBY data stored in the final merged table at 412, 443, 490, 510, 555 and 670 nm, respectively, should be used. For validation of bands 1-6 of MODIS AQUA, MOBY data stored in the final merged table at 416, 442, 489, 530, 547 and 665 nm, respectively, should be used. Finally, for validation of bands 1-7 of MERIS, MOBY data stored in the final merged table at 410.5, 440.4, 487.8, 507.7, 557.6, 617.5 and 662.4 nm, respectively, are the appropriate data.

2.2.2 BOUée pour l'acquiSition de Séries Optiques à Long termE (BOUSSOLE)

The BOUée pour l'acquiSition de Séries Optiques à Long termE (BOUSSOLE) Project started in 2001 with the objective of establishing a time series of bio-optical properties in oceanic waters to support the calibration and validation of ocean-colour satellite sensors (Antoine et al., 2006). The project is composed of a monthly cruise program and a permanent optics mooring (Antoine et al., 2008). The mooring collects radiometry and inherent optical properties (IOPs) in continuous mode every 15 minutes at 2 depths (4 and 9 m nominally). The monthly cruises are devoted to the mooring servicing, to the collection of vertical profiles of radiometry and IOPs, and to water sampling at 11 depths from the surface down to 200 m, for subsequent analyses including phytoplankton pigments, particulate absorption, coloured dissolved organic matter (CDOM) absorption and suspended particulate matter load. The BOUSSOLE mooring is in the Western Mediterranean Sea at a water depth of 2400m. All pigment (2001-2012) and radiometric (2003-2012) data were provided by the Principal Investigator. The compiled variables were "rrs" and "chla_hplc". Observations of the diffuse attenuation coefficient ("kd") were not included in the present compilation, as they were under internal quality revision at the time of data acquisition. Remote-sensing reflectance was computed from the original "fully-normalized" water-leaving radiance ("nLw_ex"), which is the "normalized" water-leaving radiance ("nLw" previously described), with a correction for the bidirectional nature of the light field (Morel and Gentili, 1996; Morel et al., 2002). The solar irradiance ("Fo") was computed from two available variables in the original set of data: the normalized water-leaving radiance ("nLw") and the remote-sensing reflectance ("rrs"), using the equation "Fo = nLw/rrs". Only radiometric observations that meet the following criteria were used: 1) tilt of the buoy was less than 10 °; 2) the buoy was not lowered by more than 2 m as compared to its nominal water line (to ensure the Es reference sensor is above water and exempt from sea spray); and 3) the solar irradiance was within 10 % of its theoretical clear-sky value (determined from Gregg and Carder, 1990). The latter criterion was used to select clear skies only. An additional quality control was to remove observations that were 50 % higher or lower than the daily average. This removed a small number of "spikes" in the time series. The final quality control step was to remove days where the standard deviation was more than half of the daily average. This was meant to identify days with high variability. Very few days (N = 2) were removed with this test. These quality control criteria were applied per wavelength, which resulted in some observations with an incomplete spectrum.

2.2.3 AErosol RObotic NETwork-Ocean Color (AERONET-OC)

The AErosol RObotic NETwork-Ocean Color (AERONET-OC) is a component of AERONET, including sites where sun-photometers operate with a modified measurement protocol leading to the determination of the fully-normalized water leaving radiance (Zibordi et al., 2006; Zibordi et al., 2009). The result of collaboration between the Joint Research Centre (JRC) and NASA, this component has been specifically developed for the validation of ocean-colour radiometric products. The strength of AERONET-OC is "the production of standardised measurements that are performed at different sites with identical measuring systems and protocols, calibrated using a single reference source and method, and processed with the same codes” (Zibordi et al., 2006; Zibordi et al., 2009). All high quality data (“Level-2”) were acquired from the project website, for 11 sites: Abu_Al_Bukhoosh (~25 °N, ~53 °E) , COVE_SEAPRISM (~36 °N, ~75 °W), Gloria (~44 °N, ~29 °E), Gustav_Dalen_Tower (~58 °N, ~17 °E), Helsinki Lighthouse (~59 °N, ~24 °E), LISCO (~40 °N, ~73 °W), Lucinda (~18 °S, ~146 °E), MVCO (~41 °N, ~70 °W), Palgrunden (~58 °N, ~13 °E), Venice (~45 °N, ~12 °E) and WaveCIS_Site_CSI_6 (~28 °N, ~90 °W). The compiled variable was “rrs”. Remote-sensing reflectance was computed from the original “fully-normalized” water-leaving radiance (see Sect. 2.2.2 for definition). The solar irradiance (“Fo”), which is not part of the AERONET-OC data, was computed from the Thuillier (2003) solar spectrum irradiance, by averaging “Fo” over a wavelength-centered 10 nm window. Data were compiled for the exact wavelengths of each record, which can change over time for a given site depending on the specific instrument deployed.

2.2.4 SeaWiFS Bio-optical Archive and Storage System (SeaBASS)

The SeaWiFS Bio-optical Archive and Storage System (SeaBASS) is one of the largest archives of in situ marine bio-optical data (Werdell and Bailey, 2003). It is maintained by NASA’s Ocean Biology Processing Group (OBPG) and includes measurements of optical properties, phytoplankton pigment concentrations, and other related oceanographic and atmospheric data. The SeaBASS database consists of in situ data from multiple contributors, collected using a variety of measurement instruments with consistent, community-vetted protocols, from several marine platforms such as fixed buoys, hand-held radiometers and profiling instruments. Quality control of the received data includes a rigorous series of protocols that range from file format verification to inspection of the geophysical data values (Werdell and Bailey, 2003). Radiometric data were acquired through the "Validation" search tool, which provided in situ data with matchups for particular ocean-colour sensors (Bailey and Werdell, 2006). The criteria in the search-query was defined to have the minimal flag conditions in the satellite data, to retrieve a greater number of matchups and therefore in situ data. Regarding phytoplankton pigment data, they were acquired through the "Pigment" search tool, which provides pigment data directly from the archives. As stated in the SeaBASS website (see “Pigment” tab at http://seabass.gsfc.nasa.gov/seabasscgi/search.cgi), the "Pigment" search tool was originally designed to return only in vitro fluorometric measurements, which is consistent with our approach, but over time chlorophyll-a measurements made using other methods (e.g. in situ fluorometry) were included in the retrieved pigment data. In the pigment data used in this work, a large number of in situ fluorometric measurements from continuous underway instruments were identified and discarded. These data were firstly identified from cruises with more than 50 observations per day, and then re-checked in the SeaBASS website to confirm whether indeed they were continuous underway measurements. A total of 148015 such measurements were identified and discarded. Given the large volume of this group of data, it is possible that some chlorophyll-a observations from in situ methods may have escaped the scrutiny and made it into the final merged data set. In the future, the SeaBASS plans to add ancillary information to the extractions, which will enable users to distinguish the different types of chlorophyll measurements. The compiled variables from SeaBASS data were: “rrs”, “chla_hplc”, “chla_fluor”, “aph”, “adg”, “bbp”, “kd”. No conversion was necessary since all variables were acquired in the desired format.

2.2.5 NASA bio-Optical Marine Algorithm Data set (NOMAD)

The NASA bio-Optical Marine Algorithm Data set (NOMAD) is a publicly-available data set compiled by the NASA OBPG at the Goddard Space Flight Center. It is a high-quality global data set of coincident radiometric and phytoplankton pigment observations for use in ocean-colour algorithm development and satellite-data product-validation activities (Werdell and Bailey, 2005). The source bio-optical data is the SeaBASS archive, therefore many dependencies exist between these two data sets, which were addressed during the merging. The current version (Version 2.0 ALPHA, 2008) includes data from 1991 to 2007 and an additional set of observations of inherent optical properties. The current version was used in this work, but with an additional set of columns of remote-sensing reflectance corrected for the bidirectional effects (Morel and Gentili, 1996; Morel et al., 2002). This additional set of columns was provided directly by the NOMAD creators. The compiled variables were “rrs”, “chla_hplc”, “chla_fluor”, “aph”, “adg”, “bbp”, “kd”. Conversion was only necessary for “aph”, “adg” and “bbp”, and followed the procedures described in Sect. 2.1. For the calculation of “bbp” the variable “bb” was used with a smooth fitting to remove noise. A portion of NOMAD data were optically weighted (for methods see Werdell and Bailey, 2005) and a small number of “chla_fluor” were from in situ fluorometry (Werdell and Bailey, 2005).These data are not consistent with the protocols chosen in this work, but these observations were retained since NOMAD is a widely-used data set in ocean-colour validation.

2.2.6 MERIS Match-up In situ Database (MERMAID)

The MERIS Match-up In situ Database (MERMAID) provides in situ bio-optical data matched with concurrent and comparable MERIS Level 2 satellite ocean-colour products (Barker, 2013a; Barker, 2013b). The MERMAID in situ database consists of data from multiple contributors, measured using a variety of instruments and protocols, from several marine platforms such as fixed buoys, hand-held radiometers and profiling instruments. Comprehensive quality control and protocols are used by MERMAID to integrate all the data into a common and comparable format (Barker, 2013a; Barker, 2013b). Access to MERMAID data is limited to the MERIS Validation Team, the MERIS Quality Working Group and to the in situ data contributors. For this work, access has been granted to the MERMAID database, through a signed Service Level Agreement. The MERMAID data includes sub-sets of several data sets used in this compilation (MOBY, AERONET-OC, BOUSSOLE, NOMAD). These observations were removed from the MERMAID dataset to avoid duplication (as discussed in Sect. 2.1). The compiled variables were “rrs”, “chla_hplc”, “chla_fluor”, “aph”, “adg”, “bbp”, “kd”. Remote-sensing reflectance was calculated by dividing by π the original irradiance reflectance provided. Conversion was also necessary for “aph”, “adg” and “bbp”, and followed the procedures described in Sect. 2.1.

2.2.7 Hawaii Ocean Time-series (HOT)

The Hawaii Ocean Time-series (HOT) programme provides repeated comprehensive observations of the hydrography, chemistry and biology of the water column at a station located 100 km north of Oahu, Hawaii, since October 1988 (Karl and

Michaels, 1996). This site is representative of the North Pacific subtropical gyre. Cruises are made approximately once a month to the deep-water Station ALOHA (A Long-Term Oligotrophic Habitat Assessment; 22° 45' N, 158° 00' W). Pigment data ("chla_hplc" and "chla_fluor") were extracted directly from the project website. Radiometric measurements from the HOT project are also available, but observations of “rrs” and “kd” from the HOT project were acquired in this work as part of the SeaBASS data set.

2.2.8 Geochemistry, Phytoplankton, and Color of the Ocean (GeP&CO)

The Geochemistry, Phytoplankton, and Color of the Ocean (GeP&CO) is part of the French PROOF programme and aims to describe and understand the variability of phytoplankton populations, and to assess its consequences on the geochemistry of the oceans (Dandonneau and Niang, 2007). It is based on the quarterly travels of the merchant ship Contship London from France to New Caledonia. A scientific observer embarked on each travel and operated the sampling for surface water, filtration, various measurements and checking at several hours of each day. The experiment started in October 1999 and finished in July 2002. Pigment data were extracted from the project website. The compiled variable was "chla_hplc".

2.2.9 Atlantic Meridional Transect (AMT)

The Atlantic Meridional Transect (AMT) is a multidisciplinary programme, which undertakes biological, chemical and physical oceanographic research during an annual voyage between the UK and destinations in the South Atlantic (Robinson et al., 2006). The programme was established in 1995 and since then has completed 23 research cruises. Pigment data between 1997 (AMT5) and 2005 (AMT17) were provided by the British Oceanographic Data Centre (BODC) following a specific request. For any interest in the original data, BODC is the point of contact, which ensures that if there are any updates, the most recent data are supplied. The compiled variables are "chla_hplc" and "chla_fluor".

2.2.10 International Council for the Exploration of the Sea (ICES)

The International Council for the Exploration of the Sea (ICES) is a network of more than 4000 scientists from almost 300 institutes, with 1600 scientists participating in activities annually. The ICES Data Centre manages a number of large data set collections related to the marine environment covering the North East Atlantic, Baltic Sea, Greenland Sea and Norwegian Sea. The majority of data originate from national institutes that are part of the ICES network of member countries. Data were provided (on 2014-04-28) from the ICES database on the marine environment (Copenhagen, Denmark) following a specific request. The ICES data were made available under the ICES data policy and if there is any conflict between this and the policy adopted by the users, then the ICES policy applies. The compiled variables were "chla_hplc" and "chla_fluor".

3 Results

In this work several sets of bio-optical in situ data were acquired, homogenised and merged into a single table. The table is comprised of in situ observations between 1997 and 2012, with a global distribution, and include the following variables: remote-sensing reflectance ("rrs"), chlorophyll-a concentration ("chla"), algal pigment absorption coefficient ("aph"), detrital and coloured dissolved organic matter absorption ("adg"), particle backscattering coefficient ("bbp") and diffuse attenuation coefficient for downward irradiance ("kd"). All observations in the table were processed in such a way that they can be compared directly with satellite-derived ocean-colour data. The table consists of 80,524 rows and 267 columns. Each row represents a unique station in space and time, separated from each other by at least 5 minutes and 200 meters. For each observation in a given station, there are three metadata strings: “dataset”, “subdataset” and “pi”. The columns of the table take the form described in Table 1. The contributors of data in the table are shown in Table 2. Regarding spectral variables, all original wavelengths were preserved, which requires a large number of unique wavelengths to be maintained in the database. No band shifting was performed (though some archived data in SeaBASS and MERMAID may have been merged with nearby wavelengths) and no minimum number of wavelengths per observation was imposed. This allows further manipulation of the table for different purposes. In the following paragraphs, the table is analysed and the final group of observations is described for each contributing data set; however, the numbers reported here do not reflect the original numbers in each data set, since duplicates across contributing data sets were removed (e.g. removed NOMAD and others from MERMAID).

Observations of remote-sensing reflectance, are available at 134 unique wavelengths (i.e. columns), between 405 nm and 1022.1 nm (Fig. 1). In total there are 44,191 observations (i.e. rows) with remote-sensing reflectance in the table. The total number of observations are partitioned per contributing data sets as follows: AERONET-OC (17,405), BOUSSOLE (17,364), MOBY (4,513), NOMAD (3,326), MERMAID (885), SEABASS (698). Data from AERONET-OC, BOUSSOLE and MOBY correspond to continuous time series, and hence the higher number of observations. Data distribution at 44X nm and 55X nm is provided in Fig. 2a and b, respectively. Data was first searched at 445 and 555 nm, and then with a search window up to 8 nm, to also include data at 547 nm. Median values at 44X nm range from 0.003 m^{-1} (AERONET-OC) and 0.009 m^{-1} (MOBY), whereas at 55X nm the median values lie between 0.001 m^{-1} (MOBY) and 0.004 m^{-1} (AERONET-OC). For additional analysis, “rrs” band ratios were plotted against each other (490:555 versus 412:443, Fig. 3). Most points are within the boundaries of the NOMAD dataset, but some scattered points were found. These points were retained in the table to allow further manipulation with different quality control criteria. Complementary analysis of remote-sensing reflectance data is made when other variables are concurrently available and discussed further on in the text (see Fig. 10 and Fig. 15). The geographic distribution of remote-sensing reflectance observations (Fig. 4) shows a higher number of observations in some coastal regions, such as those of North America and Northern Europe. The central regions of the ocean show a lower number of observations, with the Atlantic Ocean having the highest density in relation to the other oceans. Best geographic coverage is provided by the NOMAD database. Data from SeaBASS are smaller in number, but are still important. Data from MERMAID is mainly located along the coasts of Europe, North America, and the central region of the North Atlantic Ocean.

For chlorophyll-a concentration, two types of observations were compiled, one measured by fluorometric or spectrophotometric methods ("chla_fluor"), and the other measured by HPLC methods ("chla_hplc"). A comparison of both measurements, when available at the same station shows good agreement (Fig. 5). As stated before, the analysis was done on the final merged table, thus no data was filtered and the good relation can in part be explained by the quality control implemented by the data providers and curators of repositories such as NOMAD and SeaBASS (Werdell and Bailey, 2005). The total number of rows with concurrent "chla_fluor" and "chla_hplc" is 2002, with contributions from NOMAD (32 %), SeaBASS (47 %), MERMAID (11 %), HOT (7 %), AMT (2 %), GEPCO (1 %). The "chla_fluor" observations are available in 27,933 stations (rows), with values ranging from 0.0011 to 100 mg m^{-3} (Fig. 6). They are from NOMAD (2,350), SeaBASS (15,728), MERMAID (3,711), ICES (5,421), HOT (559) and AMT (164). The total number of "chla_hplc" observations is 13,918, ranging from 0.006 to 99.8 mg m^{-3} (Fig. 6), with contributions from NOMAD (1,309), SeaBASS (5,920), MERMAID (707), ICES (2,994), HOT (153), GEPCO (1,536), BOUSSOLE (397) and AMT (902). The combined chlorophyll data set (all chlorophyll data considered, but for a given station, HPLC data were selected if available), has a total of 39,849 observations, with 11 %, 41 %, 48 % respectively from oligotrophic (<0.1 mg m^{-3}), mesotrophic (0.1 - 1 mg m^{-3}), and eutrophic (>1 mg m^{-3}) waters. When compared with the proportions of the world ocean in these trophic classes, 56% oligotrophic, 42% mesotrophic and 2% eutrophic (Antoine et al., 1996), oligotrophic waters are under-represented and eutrophic waters are over-represented in the compilation. The spatial distribution of the chlorophyll values for the combined data set (Fig. 7) shows a good agreement with known biogeographical features, such has low chlorophyll values in the subtropical gyres, and high values in temperate, coastal and upwelling regions. Many regions show a good spatial coverage (e.g. Atlantic and Pacific Ocean), while others are poorly sampled (e.g. Southern and Indian Oceans). Of the contributing data sets, NOMAD and SeaBASS provide a good spatial coverage in many regions (Fig. 8). The ICES and MERMAID data are mainly located along the coastal regions of Europe. The AMT data covers the central part of the Atlantic Ocean. For additional analysis and as an example of the applications of the compiled data set, the combined chlorophyll data ("chla_fluor" and "chla_hplc") were partitioned into 5º x 5º boxes and for each box the number of observations, average value and standard deviation were computed (Fig. 9 a, b and c, respectively). The number of observations can be very high (>1000) in some boxes along the European and North American coastlines and relatively low (<20) in oceanic regions. Again there is an appearance in the average value map (Fig. 9 b) of well-known biogeographical features, such has the lower chlorophyll in the subtropical gyres and high values in coastal and upwelling areas. There is a close correspondence between the spatial patterns of the averaged and standard deviation maps (Fig. 9 b and c), which may be an indicator of the data quality.

Coincident observations of chlorophyll-a concentration and remote-sensing reflectance are available at 3,562 stations. These observations are mostly from NOMAD (85 %), MERMAID (10 %) and SeaBASS (5 %). The maximum of three band ratios of remote-sensing reflectance is plotted against chlorophyll-a concentration (Fig. 10). The "chla" values used are the combined HPLC and fluorometric chlorophyll-a and for the "rrs", the closest spectral observation within 2 nm was used. The maximum band ratios were calculated using the maximum value between [rrs(443)/rrs(555), rrs(490)/rrs(555), rrs(510)/rrs(555)] or [rrs(443)/rrs(560), rrs(490)/rrs(560), rrs(510)/rrs(560)] if rrs(555) was not available. The relationship between maximum band ratio and chlorophyll is close to the NASA OC4 and OC4E v6 standard algorithm (http://oceancolor.gsfc.nasa.gov/cms/atbd/chlor_a) based on maximum band ratios, providing confidence in the quality of the compiled data.

The inherent optical properties (“aph”, “adg” and “bbp”) are available at 27 unique wavelengths between 405 and 683 nm. There are a total of 1,276, 1,123 and 638 observations, for “aph”, “adg” and “bbp”, respectively. For “aph” the total number of observations is distributed among NOMAD (1,190), SeaBASS (14) and MERMAID (72). For “adg” the contributions are as follows: NOMAD (1,079), SeaBASS (11) and MERMAID (33). The “bbp” observations come from NOMAD (371), SeaBASS (32) and MERMAID (235). Data distribution of “aph”, “adg” and “bbp” at 44X nm and 55X nm for each data set is provided in Fig. 11 a - f. Median values of “aph”, “adg” and “bbp” at 44X and 55X nm for each data set are summarized in Table 3. For additional analysis, the following band ratios for the absorption coefficients were calculated: aph(490)/aph(443), aph(412)/aph(443), adg(443)/adg(490) and adg(412)/adg(443). Data within 2 nm of the wavelengths were used to maximize the number of points. The distribution of the ratios is shown in Fig. 12. Several observations were found to be above the thresholds used in the IOCCG report 5 for quality control (see dotted vertical black lines in Fig. 12). These points are highlighted here for information, but retained in the database, as these were mostly from NOMAD and there was an interest to preserve this data set as a whole. Also not discarding this data allows further manipulation with different quality control criteria. The geographic coverage for observations of “aph”, “adg” and “bbp” (Fig. 13) is poor, with most open ocean regions not being sampled, with the exception of the Atlantic Ocean. Small clusters of data are located in particular coastal regions.

Finally, for the diffuse attenuation coefficient for downward irradiance ("kd") there are 25 unique wavelengths between 405 and 709 nm. There are a total of 2,454 observations, from NOMAD (2,266), SeaBASS (118) and MERMAID (70). Data distribution of “kd” at 44X nm and 55X nm for each data set is shown in Fig. 11 g and h. No “kd” data at these wavelengths were available for the SeaBASS data set (only at 490 nm). Median values of “kd” at 44X nm span between 0.08 m^{-1} (NOMAD) to 0.1 m^{-1} (MERMAID), whereas at 55X nm the “kd” values are approximately 0.1 m^{-1} (NOMAD and MERMAID). The NOMAD provides the best geographic coverage (Fig. 14), with a higher coverage in the Atlantic, compared with other oceans. With the exception of the coastal regions of North America and the Japan Sea, most coastal regions are not sampled.

Although most of the stations with concurrent variables are mainly from the NOMAD data set, for completeness, an examination of bio-optical relationships is provided (Fig. 15). The relation between “aph” at 443 nm and chlorophyll-a (Fig. 15 a) agrees with the relation proposed by Bricaud et al. (2004). A total number of 1,070 points exists with these two variables available (93 % from NOMAD). The relation between the sum of “aph” and “adg” at 443 nm and “rrs” at 443 nm (Fig. 15 b), shows a similar dispersion, with the exception of some scattered points, to an equivalent analysis on the IOCCG report 5

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(see their Fig. 2.3). Again, the scattered data were retained in the final table to preserve the NOMAD data set. A total number of 1112 points exist for which these three variables available (97 % from NOMAD). The relation between the ratio rrs(490)/rrs(555) and kd(490) (Fig. 15 c) shows a good agreement with the NASA KD2S standard algorithm (http://oceancolor.gsfc.nasa.gov/cms/atbd/kd_490). A total number of 2,280 points exist for which these three variables are available (93 % from NOMAD). The relation between the ratio rrs(490)/rrs(555) and "bbp" at 555 nm (Fig. 15 c) shows a good agreement with the relation suggested by Tiwari and Shanmugam (2013). A total number of 357 points exist for which these three variables are available (91 % from NOMAD).

The merged text table described in this work, considered here as the main table, is accompanied by 4 extra files. One extra file is a "csv" table with detailed information about the number of observations per variable, "dataset", "subdataset" and "pi". Two other extra files are text tables generated from the main table, and are provided to help with the analysis of spectral data. These two files contain the spectral data aggregated within +-2 nm and +-6 nm, respectively, of SeaWiFS, MODIS AQUA and MERIS sensor bands. The files are generated by assigning, in each row of the main table, the closest spectral observation within 2 nm (or 6 nm) of a sensor band. The centre-wavelength of each band and sensor used in the generation of the files are the following: SeaWiFS bands 1-8 were centred at [412, 443, 490, 510, 555, 670, 765, 865] nm, respectively; MODIS-AQUA bands 1-9 were centred at [412, 443, 488, 531, 547, 667, 678, 748, 869] nm, respectively; MERIS bands 1-13 were centred at [412, 442, 490, 510, 560, 620, 665, 681, 709, 753, 779, 865, 885] nm, respectively. An exception to this procedure was made to confirm that the correct MOBY data are stored in the files (see Sect. 2.2.1. for discussion on how MOBY wavelengths are stored in the main file). Finally, a "readme" file is provided to help the user.

4 Conclusion

A compilation of bio-optical in situ data is presented in this work. The compiled data have a global coverage and spans from 1997 to 2012, covering the recent period of ocean-colour satellite observations. It resulted from the acquisition, homogenization and integration of several sets of data obtained from different sources. Minimum changes were made on the original data, other than the ones occurring from conversion to standard format and quality control. In situ measurements of the following variables were compiled: remote-sensing reflectance, chlorophyll-a concentration, algal pigment absorption coefficient, detrital and coloured dissolved organic matter absorption coefficient, particle backscattering coefficient and diffuse attenuation coefficient for downward irradiance.

The final set of data consists of a substantial number of in situ observations, available in a simple text table, and processed in a way that could be used directly for the evaluation of satellite-derived ocean-colour data. The major advantages of this compilation is that it merges six commonly-used data sources in ocean-colour validation (MOBY, BOUSSOLE, AERONET-OC, SeaBASS, NOMAD, MERMAID), and four additional sets of chlorophyll-a concentration data (AMT, ICES, HOT and GEPCO) into a simple text table free of duplicated observations. This compilation was initially created with the intention of evaluating the quality of the satellite ocean-colour products from the ESA OC-CCI project. The objective of publishing the compilation is to make it easy for the broader community to use it.

Author contribution

The first six authors belong to the ESA OC-CCI team and contributed to the design of the compilation. The remaining authors are listed alphabetically and are data contributors (see their respective data set on Table 2) or individuals responsible for the development of a particular data set (Jeremy Werdell for NOMAD and Katherine Barker for MERMAID). All data contributors (listed on Table 2) were contacted for authorization of data publishing and offered co-authorship. In the case of the ICES data set the permission for publishing was given by the ICES team. All the authors have critically reviewed the manuscript.

APENDIX A: Notation

ad	Detrital absorption coefficient (m^{-1})
adg	Detrital plus CDOM absorption coefficient (m^{-1})
AERONET-OC	AErosol RObotic NETwork-Ocean Color
ag	CDOM absorption coefficient (m^{-1})
AMT	Atlantic Meridional Transect
ap	Particle absorption coefficient (m^{-1})
aph	Algal pigment absorption coefficient (m^{-1})
aw	Pure water absorption coefficient (m^{-1})
bb	Total backscattering coefficient (m^{-1})
bbp	Particle backscattering coefficient (m^{-1})
bbw	Backscattering coefficient of seawater (m^{-1})
BOUSSOLE	Bouée pour l’acquisition d'une Série Optique à Long Terme
CDOM	Coulored Dissolved Organic Matter
chla	Chlorophyll a concentration (mg m^{-3})
chla_fluor	Chlorophyll a concentration determined from fluorometric or spectrophotometric methods (mg m^{-3})
chla_hplc	Total chlorophyll a concentration determined from HPLC method (mg m^{-3})
Es	Surface irradiance (or above-water downwelling irradiance) (mW cm^{-2} µm^{-1})
ESA	European Space Agency
Fo	Top-of-the-atmosphere solar irradiance (mW cm^{-2} µm^{-1})
GeP&CO	Geochemistry, Phytoplankton, and Color of the Ocean
HOT	Hawaii Ocean Time-series
HPLC	High-Performance Liquid Chromatography

ICES	International Council for the Exploration of the Sea
kd	Diffuse attenuation coefficient for downward irradiance (m^{-1})
Lw	water-leaving radiance (or above-water upwelling radiance) (mW cm^{-2} µm^{-1} sr^{-1})
MERIS	Medium Resolution Imaging Spectrometer
MERMAID	MERIS Match-up In situ Database
MOBY	Marine Optical Buoy
MODIS	Moderate Resolution Imaging Spectro-radiometer
NASA	National Aeronautics and Space Administration
nLw	Normalized water-leaving radiance (mW cm^{-2} µm^{-1} sr^{-1})
nLw_ex	nLw with a correction for bidirectional effects (mW cm^{-2} µm^{-1} sr^{-1})
NOMAD	NASA bio-Optical Marine Algorithm Data set
OC-CCI	Ocean Colour Climate Change Initiative
rrs	Remote-sensing reflectance (sr^{-1})
SeaBASS	SeaWiFS Bio-optical Archive and Storage System
SeaWiFS	Sea-viewing Wide Field-of-view Sensor
Rw	Irradiance reflectance (dimensionless)

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Manuscript under review for journal Earth Syst. Sci. Data
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FIGURES & TABLES

Variable/Column	Description and units
time	GMT, <YYYY-MM-DD>T<HH:MM:SS>Z
lat	Decimal degree, -90:90, South Negative
lon	Decimal degree, -180:180, West Negative
chla_hplc	Total chlorophyll a concentration determined from HPLC method (mg m^{-3})
chla_fluor	Chlorophyll a concentration determined from fluorometric or spectrophotometric methods (mg m^{-3})
rrs_<band>	Remote-sensing reflectance (sr^{-1})
aph_<band>	Algal pigment absorption coefficient (m^{-1})
adg_<band>	Detrital plus CDOM absorption coefficient (m^{-1})
bbp_<band>	Particle backscattering coefficient (m^{-1})
kd_<band>	Diffuse attenuation coefficient for downward irradiance (m^{-1})
etopo1	Water depth from ETOPO1 (m)
chla_hplc_dataset	Metadata string for "chla_hplc"
chla_hplc_subdataset	Metadata string for "chla_hplc"
chla_hplc_pi	Metadata string for "chla_hplc"
chla_fluor_dataset	Metadata string for "chla_fluor"
chla_fluor_subdataset	Metadata string for "chla_fluor"
chla_fluor_pi	Metadata string for "chla_fluor"
rrs_dataset	Metadata string for "rrs"
rrs_subdataset	Metadata string for "rrs"
rrs_pi	Metadata string for "rrs"
aph_dataset	Metadata string for "aph"
aph_subdataset	Metadata string for "aph"
aph_pi	Metadata string for "aph"
adg_dataset	Metadata string for "adg"
adg_subdataset	Metadata string for "adg"
adg_pi	Metadata string for "adg"
bbp_dataset	Metadata string for "bbp"
bbp_subdataset	Metadata string for "bbp"
bbp_pi	Metadata string for "bbp"
kd_dataset	Metadata string for "kd"
kd_subdataset	Metadata string for "kd"
kd_pi	Metadata string for "kd"

Table 1: The standard variables, nomenclatures and units in the final table.

Data Source	Description	Data contributors
Marine Optical Buoy (MOBY)	Daily observations of remote-sensing reflectance, measured by a fixed mooring system, located west of the Hawaiian Island of Lanai. Data compiled between 1997-2012. Data were obtained from the MOBY website. Compiled standard variable: “rrs”.	Paul DiGiacomo, Kenneth Voss
Bouée pour l’acquisition d'une Série Optique à Long Terme (BOUSSOLE)	High frequency (15 min) observations of remote-sensing reflectance, from a fixed mooring system, located in the Western Mediterranean Sea. Measurements of chlorophyll-a concentration are also available at the mooring locations. Remote-sensing reflectance and chlorophyll-a data were compiled between 2003-2012 and 2001-2012, respectively. Data were provided by David Antoine. Compiled standard variables: “rrs”, “chla_hplc”.	David Antoine
AErosol RObotic NETwork-Ocean Color (AERONET-OC)	Daily observations of remote-sensing reflectance, measured by modified sun-photometers. Data compiled between 2002-2012. Sites included: Abu_Al_Bukhoosh (~25 °N, ~53 °E) , COVE_SEAPRISM (~36 °N, ~75 °W), Gloria (~44 °N, ~29 °E), Gustav_Dalen_Tower (~58 °N, ~17 °E), Helsinki Lighthouse (~59 °N, ~24 °E), LISCO (~40 °N, ~73 °W), Lucinda (~18 °S, ~146 °E), MVCO (~41 °N, ~70 °W), Palgrunden (~58 °N, ~13 °E), Venice (~45 °N, ~12 °E), WaveCIS_Site_CSI_6 (~28 °N, ~90 °W). Data were obtained from the AERONET-OC website. Compiled standard variable: “rrs”.	Robert Arnone [WaveCIS], Sam Ahmed [LISCO], Vittorio Brando [Lucinda], Dick Crout [WaveCIS], Hui Feng [MVCO], Alex Gilerson [LISCO], Rick Gould [WaveCIS], Brent Holben [COVE-SEAPRISM], Susanne Kratzer [Palgruden], Heidi M. Sosik [MVCO], Giuseppe Zibordi [Abu Al Bukhoosh & Gloria & Gustav Dalen Tower & Helsinki Lighthouse & Venice]
SeaWiFS Bio-optical Archive and Storage System (SeaBASS)	Global archive of in situ marine data from multiple contributors. Bio-optical global data between 1997-2012 were extracted from the SeaBASS website. Pigment data were extracted using "Data Search" tool, which provides data directly from the archives. Radiometric data were extracted using "Validation" tool, which only provides in situ data with matchups for ocean colour sensors. Compiled standard variables: “rrs”, “chla_hplc”, “chl_fluor”, “aph”, “adg”, “bbp”, “kd”.	Robert Arnone, Kevin Arrigo, William Balch, Ray Barlow, Mike Behrenfeld, Sukru Besiktepe, Emmanuel Boss, Chris Brown, Douglas Capone, Ken Carder, Francisco Chavez, Alex Chekalyuk, Jay-Chung Chen, Dennis Clark, Herve Claustre, Jorge Corredor, Glenn Cota, Yves Dandonneau, Heidi Dierssen, David Eslinger, Piotr Flatau, Robert Frouin, Carlos Garcia, Joaquim Goes, Gwo-Ching Gong, Rick Gould, Larry Harding, Jon Hare, Stan Hooker, Chuanmin Hu, Sung-

		Ho Kang, Gary Kirkpatrick, Oleg Kopelevich, Sam Laney, Zhongping Lee, Ricardo Letelier, Marlon Lewis, Antonio Mannino, John Marra, Chuck McClain, Christophe Menkes, Mark Miller, Greg Mitchell, Ru Morrison, James Mueller, Frank Muller-Karger, James Nelson, Norman Nelson, Mary Jane Perry, David Phinney, John Porter, Collin Roesler, David Siegel, Mike Sieracki, Jeffrey Smart, Raymond Smith, Heidi Sosik, James Spinhirne, Dariusz Stramski, Rick Stumpf, Ajit Subramaniam, Chuck Trees, Michael Twardowski, Kenneth Voss, Marcel Wernand, Ronald Zaneveld, Eric Zettler, Giuseppe Zibordi, Richard Zimmerman
NASA bio-Optical Marine Algorithm Data set (NOMAD)	High-quality global data set of coincident bio-optical in situ data. The data set was build upon SeaBASS archive. It was used the current version (Version 2.0 ALPHA, 2008) with an additional set of columns of remote-sensing reflectance corrected for the bidirectional nature of the light field, provided by NOMAD creators. Data compiled between 1997-2007. Compiled standard variables: “rrs”, “chla_hplc”, “chl_fluor”, “aph”, “adg”, “bbp”, “kd”.	Robert Arnone, Kevin Arrigo, William Balch, Ray Barlow, Mike Behrenfeld, Chris Brown, Douglas Capone, Ken Carder, Francisco Chavez, Dennis Clark, Herve Claustre, Jorge Corredor, Glenn Cota, David Eslinger, Piotr Flatau, Robert Frouin, Rick Gould, Larry Harding, Stan Hooker, Oleg Kopelevich, Marlon Lewis, Antonio Mannino, John Marra, Mark Miller, Greg Mitchell, Tiffany Moisan, Ru Morrison, Frank Muller-Karger, James Nelson, Norman Nelson, David Siegel, Raymond Smith, Timothy Smyth, James Spinhirne, Dariusz Stramski, Rick Stumpf, Ajit Subramaniam, Kenneth Voss
MERIS Match-up In situ Database (MERMAID)	Global database of in situ bio-optical data matched with concurrent MERIS Level 2 satellite ocean colour products. It was used the "Extract matchup" tool to acquire data. Data was compiled between 2002-2012. Access has been granted through a signed Service Level Agreement. Compiled standard variables: “rrs”, “chla_hplc”, “chl_fluor”, “aph”, “adg”, “bbp”, “kd”.	Simon Belanger, Jean-Francois Berthon, Vanda Brotas, Elisabetta Canuti, Pierre Yves Deschamps, Annelies Hommersom, Mati Kahru, Holger Klein, Hubert Loisel, David McKee, Greg Mitchell, Michael Ondrusek, Michel Repecaud, David Siegel, Giuseppe Zibordi
Atlantic Meridional Transect (AMT)	Multidisciplinary programme that makes biological, chemical and physical oceanographic measurements during an annual voyage between	Ray Barlow, Stuart Gibb, Victoria Hill, Patrick Holligan, Gerald Moore, Leonie O'Dowd, Alex Poulton, Emilio Suarez

	the United Kingdom and destinations in the South Atlantic. It has compiled observations of chlorophyll-a concentration between 1997 (AMT5) and 2005 (AMT17). Data were provided by the British Oceanographic Data Centre (BODC). Compiled standard variables: "chla_hplc", "chl_fluor".	
International Council for the Exploration of the Sea (ICES)	Database of several collections of data related to the marine environment. It has compiled observations of chlorophyll-a concentration in the northern European Seas, between 1997-2012. Data were provided by the ICES database on the marine environment (2014, Copenhagen, Denmark). Compiled standard variables: "chla_hplc", "chl_fluor".	Not Available
Hawaii Ocean Time-series (HOT)	Multidisciplinary programme that makes repeated biological, chemical and physical oceanographic observations near Oahu, Hawaii. Measurements of chlorophyll-a concentration between 1997-2012 were extracted from the project website. Compiled standard variables: "chla_hplc", "chl_fluor".	Bob Bidigare, Matthew Church, Ricardo Letelier, Jasmine Nahorniak
Geochemistry, Phytoplankton, and Color of the Ocean (GeP&CO)	Program of in situ data collection aboard merchant ship from France to New Caledonia, between 1999 and 2002. Measurements of chlorophyll-a concentration were obtained from the project website. Compiled standard variables: "chla_hplc".	Yves Dandonneau

Table 2: Original sets of data and data contributors in the final table.

	Median "aph"		Median "adg"		Median "bbp"	
	44x nm	55x nm	44x nm	55x nm	44x nm	55x nm
seabass	0.0549	0.0074	0.0711	0.0222	0.0035	0.0025
mermaid	0.0353	0.0046	0.0515	0.0112	0.0030	0.0022
nomad	0.0282	0.0052	0.1149	0.0286	0.0080	0.0052

Table 3. Summary of median values for "aph", "adg" and "bbp" at 44X and 55X nm for each data set (as shown in Fig. 11 a-f). Data was first searched at 445 and 555 nm, and then with a search window up to 8 nm, to include data at 547 nm.

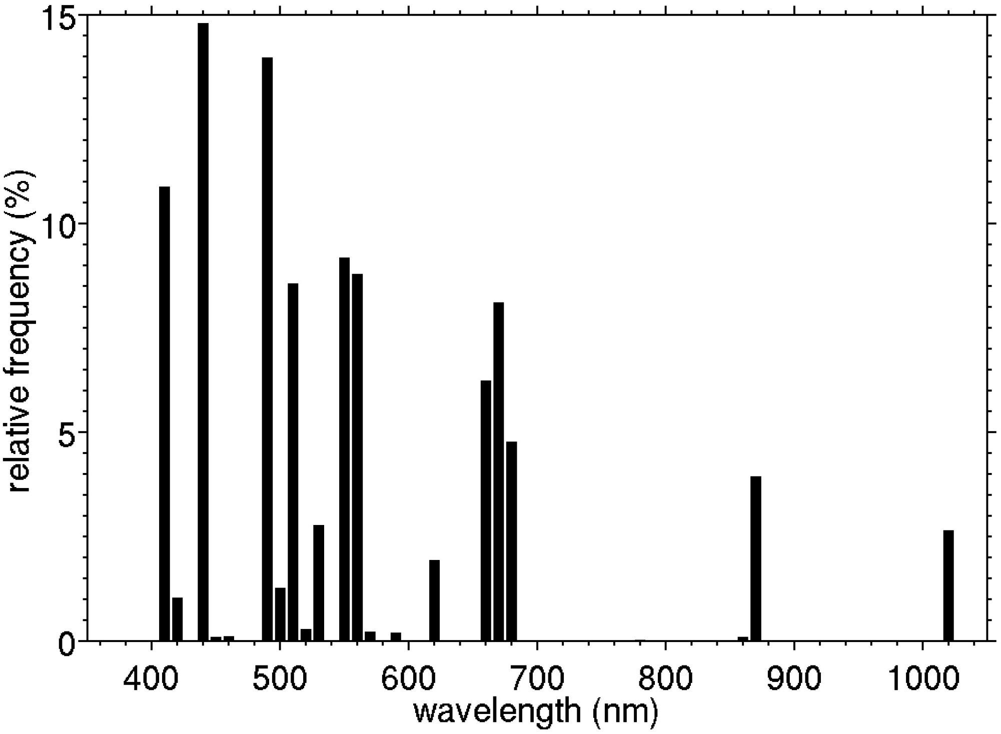

Figure 1. Relative spectral frequency of remote-sensing reflectance in the final table, using 10 nm wide class intervals, defined as the ratio of the number of observations at a particular waveband to the total number of observations at all wavebands, multiplied by 100 to report results in percentage. Data at a total of 134 unique wavelengths, between 405 nm and 1022.1 nm, were compiled.

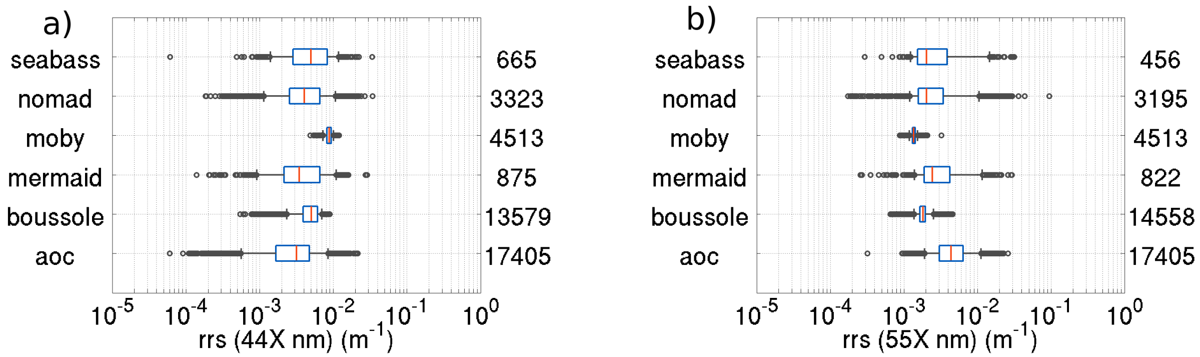

Figure 2. The distribution of (a) “rrs” at 44X nm and (b) “rrs” at 55X nm. Data was first searched at 445 and 555 nm, and then with a search window of up to 8 nm, to include data at 547 nm. The black boxes delimit the percentiles 0.25 and 0.75 of the data and the black horizontal lines show the extension of up to percentiles 0.05 and 0.95. The red line represents the median value and the black circles the values below (and above) the percentile 0.05 (0.95). The number of measurements of each data set is reported on the right axis of the graph.

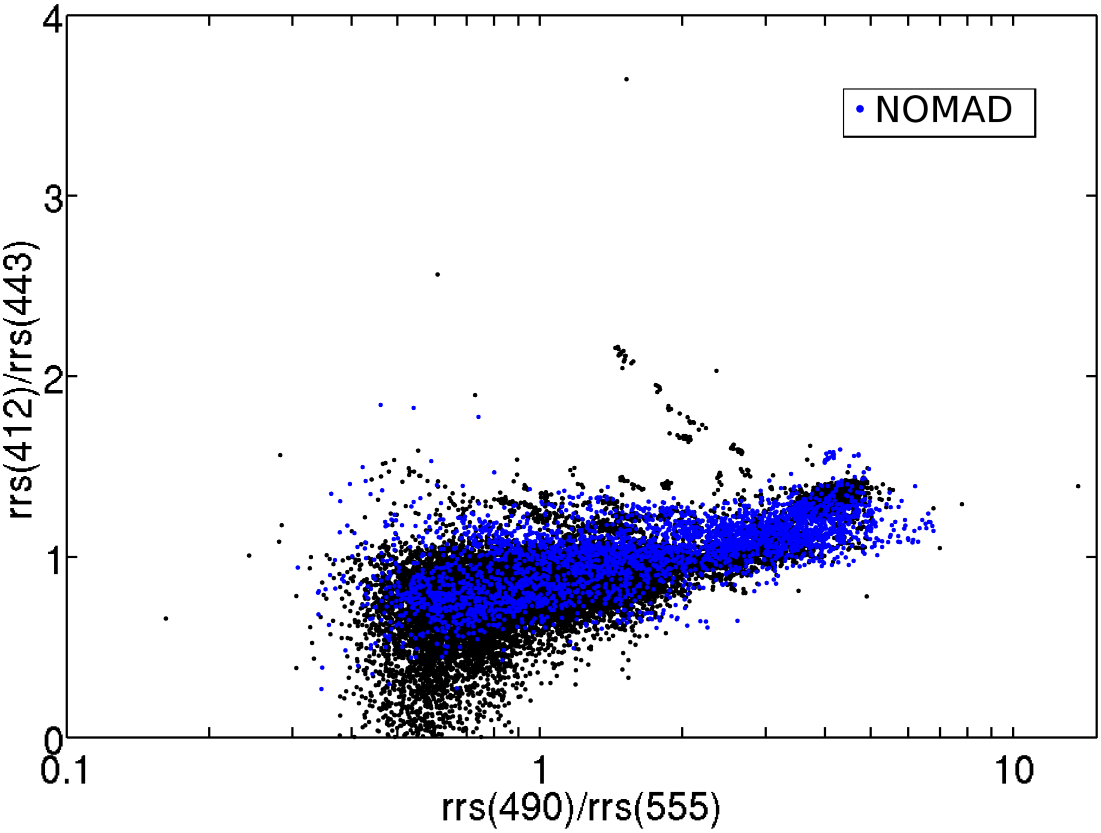

Figure 3. Ranges of remote-sensing reflectance band ratios (412:443 and 490:555) for all data. The points from the NOMAD data set are shown in blue for reference. The total number of points is divided between MOBY (4,513), AERONET-OC (17,293), BOUSSOLE (3,533), NOMAD (3,120), SeaBASS (432) and MERMAID (677). To maximize the number of ratios per data set a search window up to 12 nm was used, when the four wavelengths (412, 443, 490, 555) were not simultaneous available. The effect of different search windows was negligible in the ratio distribution.

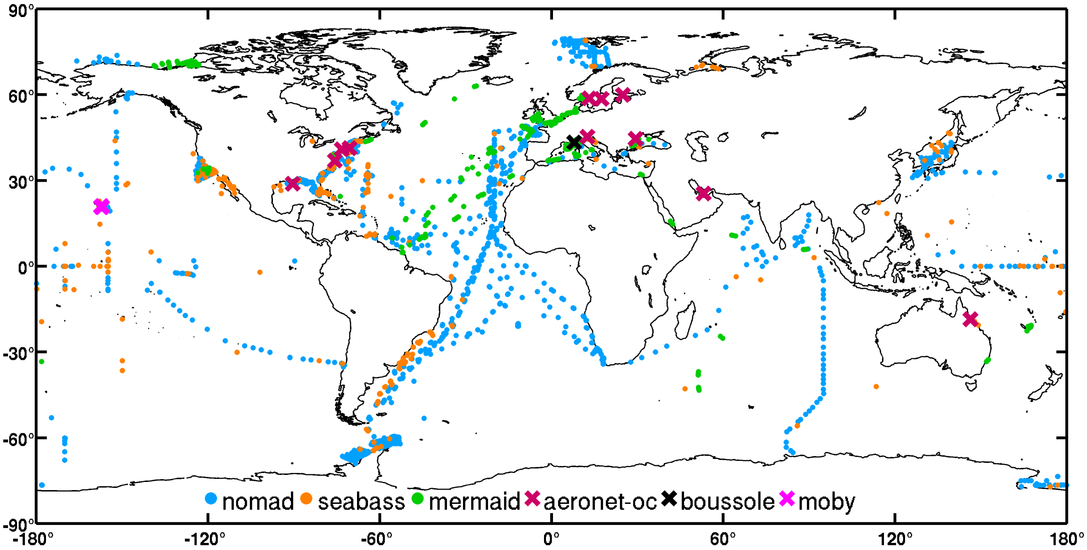

Figure 4. Global distribution of remote-sensing reflectance per data set in the final table. The data sources are identified with different colours. Points show locations where at least one observation is available. Crosses show sites from where time series data of remote-sensing reflectance are available.

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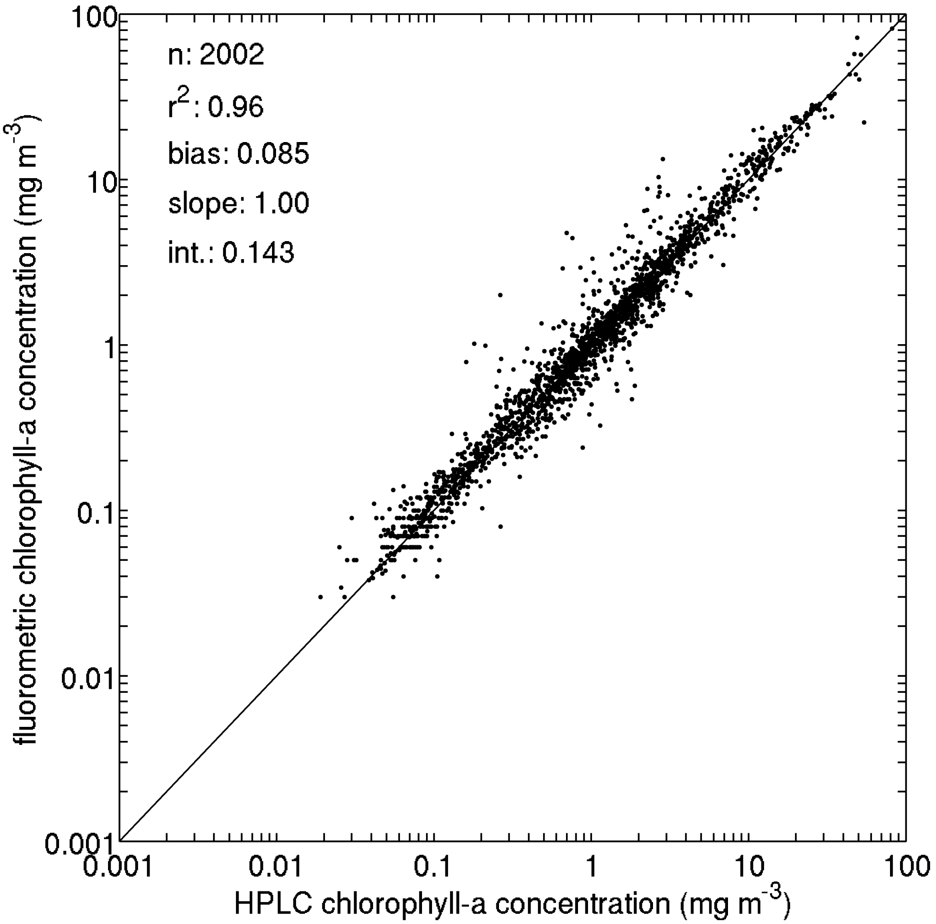


Figure 5. Comparison of coincident observations of chlorophyll-a concentration derived with different methods (“chla_fluor” and “chla_hplc”). The data were transformed prior to regression analysis to account for their log-normal distribution.

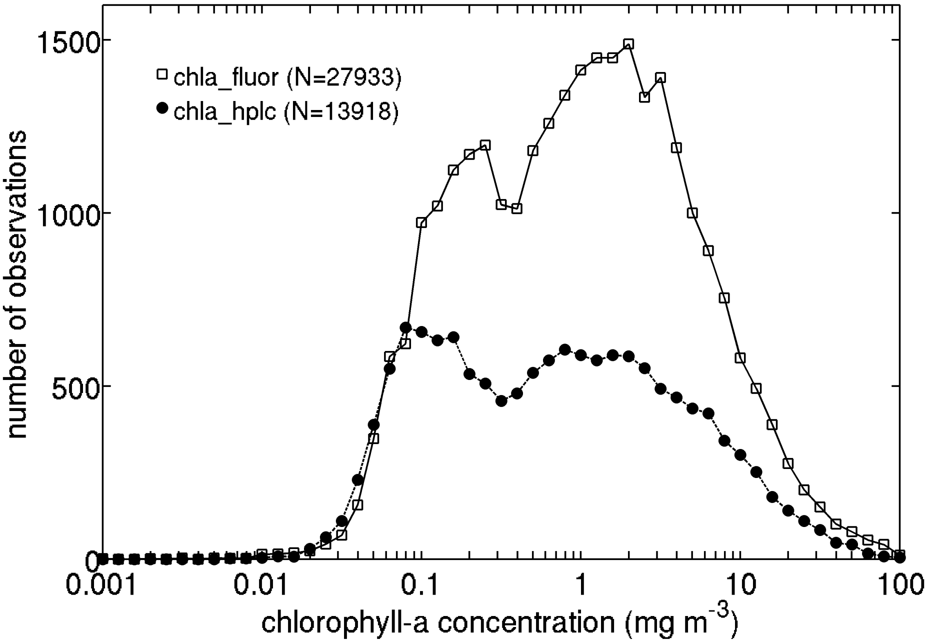


Figure 6. Number of observations per chlorophyll-a concentration acquired with different methods (“chla_fluor” and “chla_hplc”).

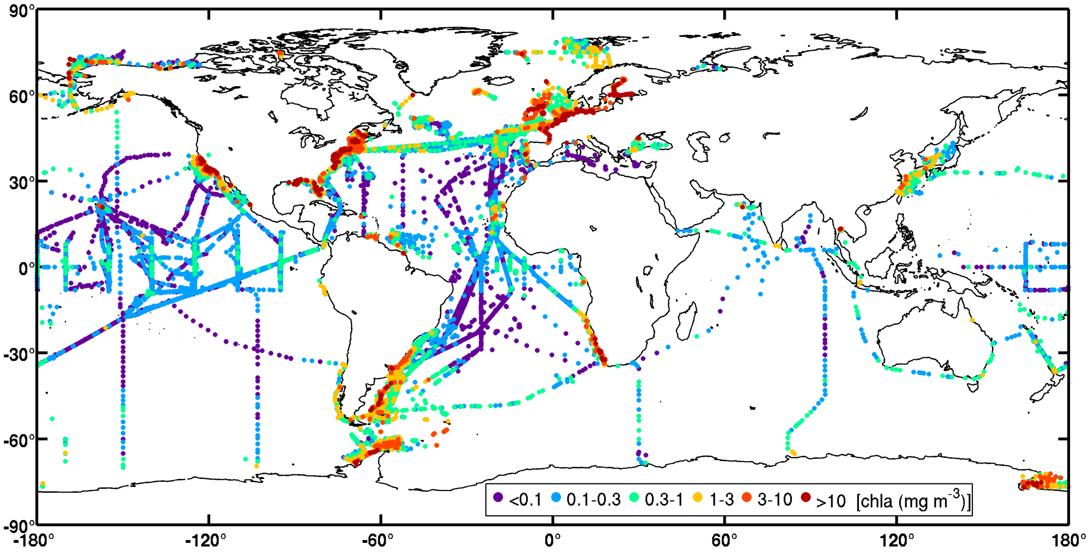
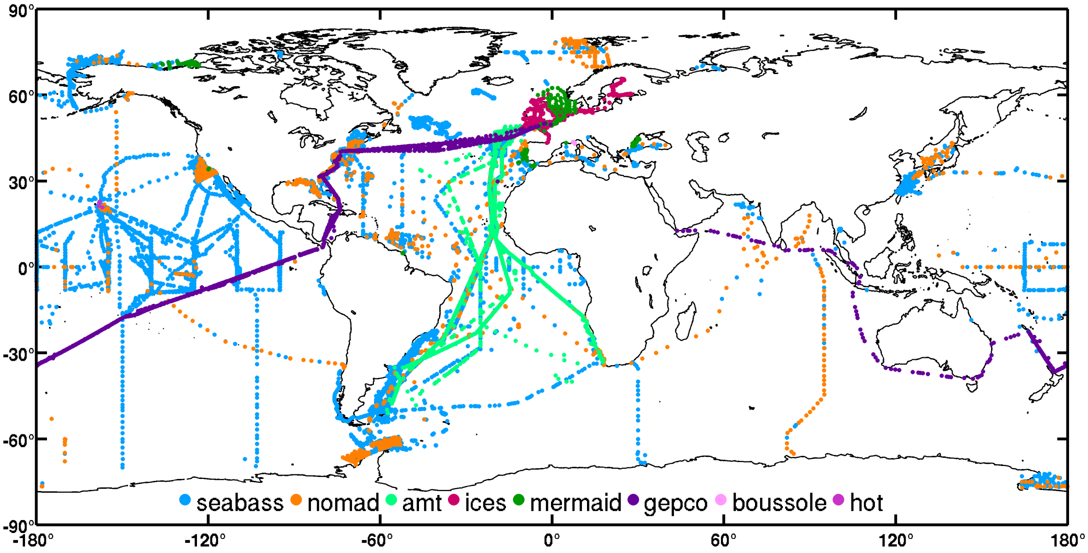

90°
60°
30°
0°
-30°
-60°
-90°
-180°
-120°
-60°
0°
60°
120°
180°
● <0.1 ● 0.1-0.3 ● 0.3-1 ● 1-3 ● 3-10 ● >10 [chla (mg m^{-3})]

Figure 7. Global distribution of chlorophyll-a concentration per intervals of the observed value. All chlorophyll data were considered, but for a given station, HPLC data were selected if available.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-60°
0°
60°
120°
180°
● seabass ● nomad ● amt ● ices ● mermaid ● gepco ● boussole ● hot

Figure 8. Global distribution of chlorophyll-a concentration per data set in the final table. All chlorophyll data were considered, but for a given station, HPLC data were selected if available.

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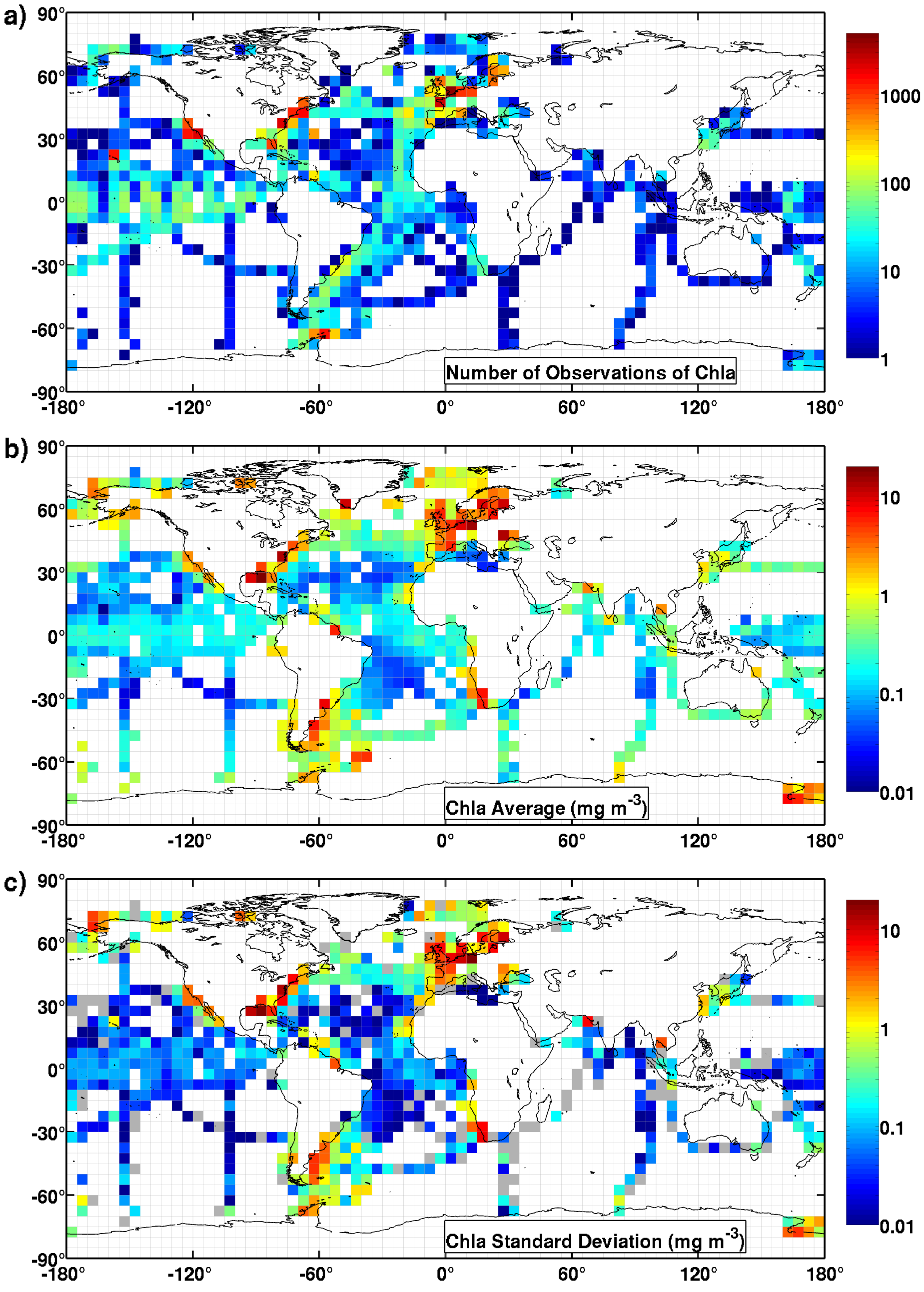

Figure 9. The chlorophyll-a (mg m^{-3}) data partitioned into 5º x 5º boxes showing the (a) number of observations, (b) average value and (c) standard deviation in each box. All chlorophyll data were considered, but for a given station, HPLC data were selected if available. In the standard deviation plot, grey colour boxes represent boxes with zero standard deviation (i.e. one
5 observation).

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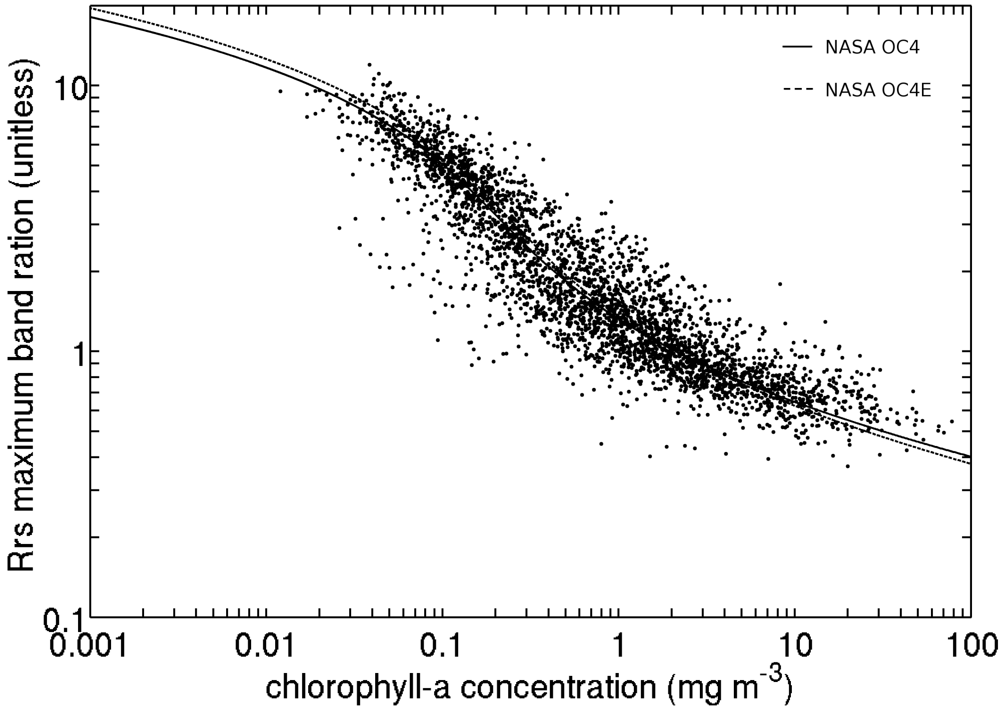

Figure 10. A remote-sensing reflectance maximum band ratio ([443,490,510]/555 or [443,490,510]/560 if 555 not available) as a function of chlorophyll-a concentration. All chlorophyll data were considered, but for a given station, HPLC data were selected if available. Data within 2 nm of the wavelengths were used. For reference the solid and dotted line show the NASA OC4 and OC4E v6 standard algorithms, respectively (http://oceancolor.gsfc.nasa.gov/cms/atbd/chlor_a). The total number of points was 3,369, of which 86% were from NOMAD.

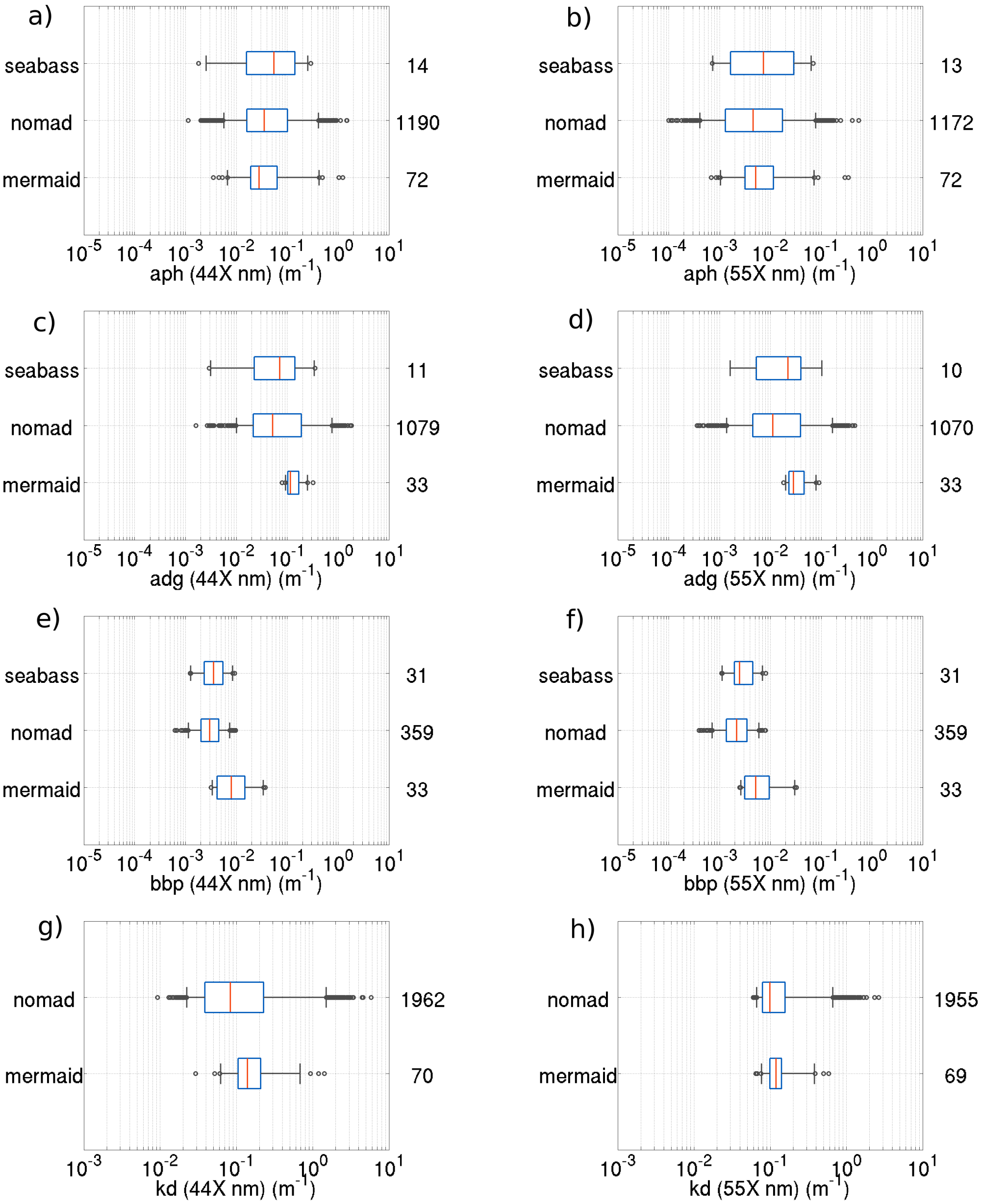

Figure 11. The distribution of (a) "aph" at 44X nm; (b) "aph" at 55X; (c) "adg" at 44X nm; (d) "adg" at 55X; (e) "bbp" at 44X nm; (f) "bbp" at 55X; (g) "kd" at 44X nm; (h) "kd" at 55Xnm. Data was first searched at 445 and 555 nm, and then with a search window up to 8 nm, to include data at 547 nm. The graphical convention is identical to Fig. 2.

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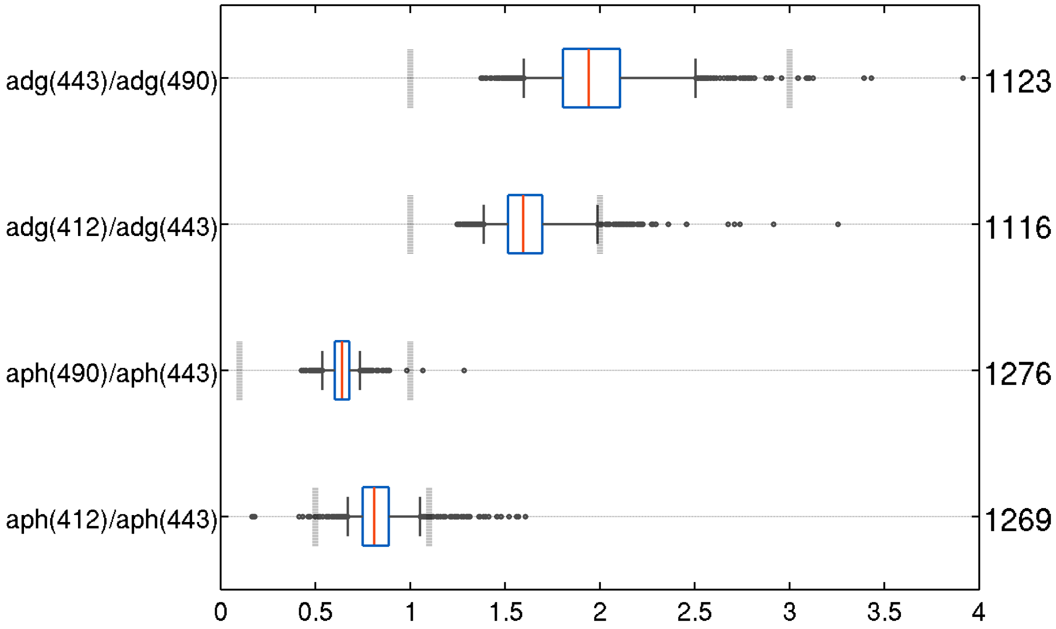

5 Figure 12. The distribution of absorption coefficients band ratios: adg(443)/adg(490), adg(412)/adg(443), aph(490)/aph(443) and aph(412)/aph(443). Data within 2 nm of the wavelengths were used. The graphical convention is identical to Fig. 2. The vertical dashed lines show the lower and upper thresholds used for quality control in the IOCCG report 5. The total number of points are divided between NOMAD (93-96%), MERMAID (3-6%) and SeaBASS (1%).

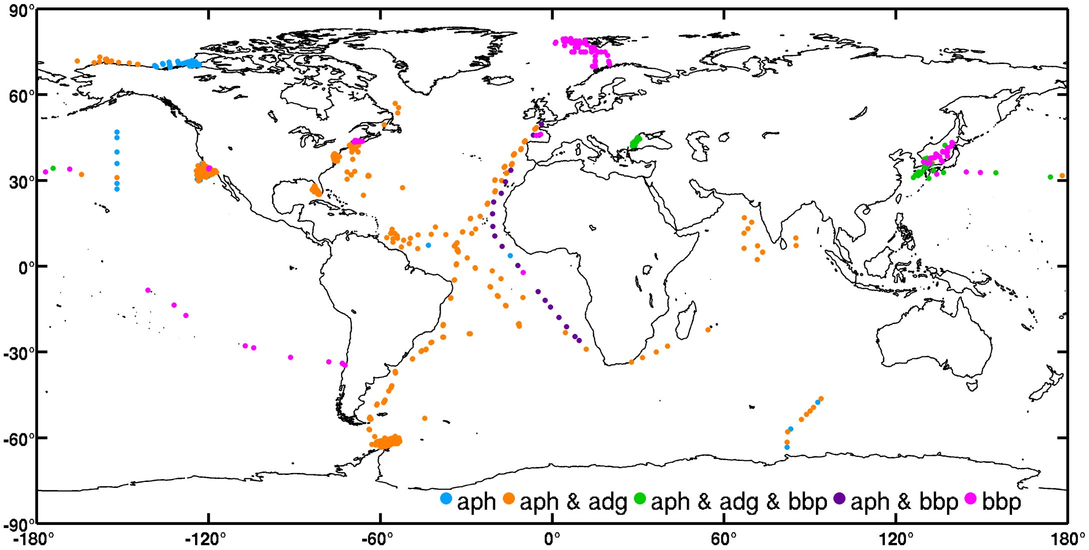

Figure 13. Global distribution of observations of inherent optical properties (algal pigment absorption coefficient “aph”, detrital plus CDOM absorption coefficient “adg” and particle backscattering coefficient “bbp”) in the final table.

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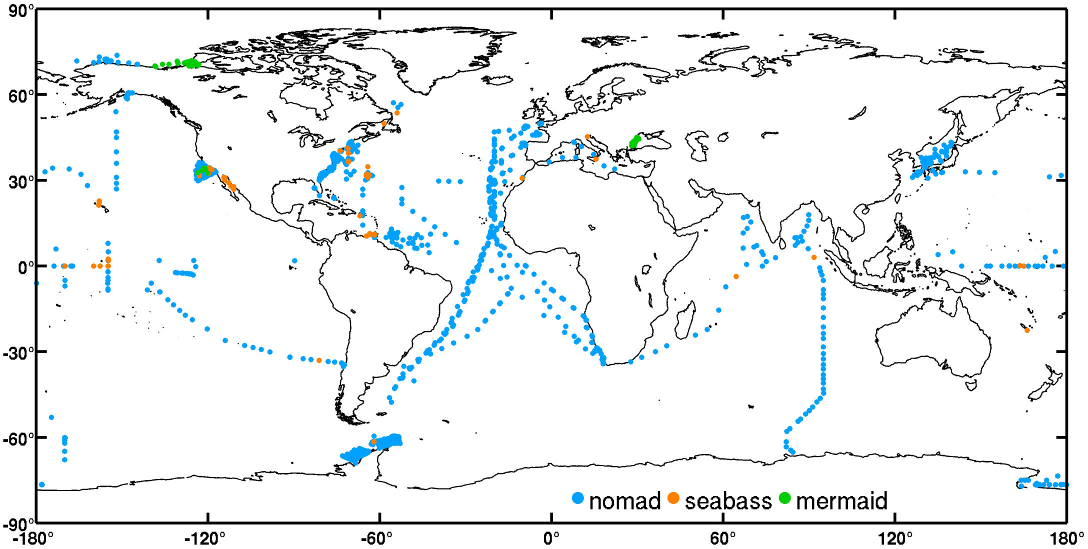

Figure 14. Global distribution of diffuse attenuation coefficient for downward irradiance (kd”) per data set in the final table.

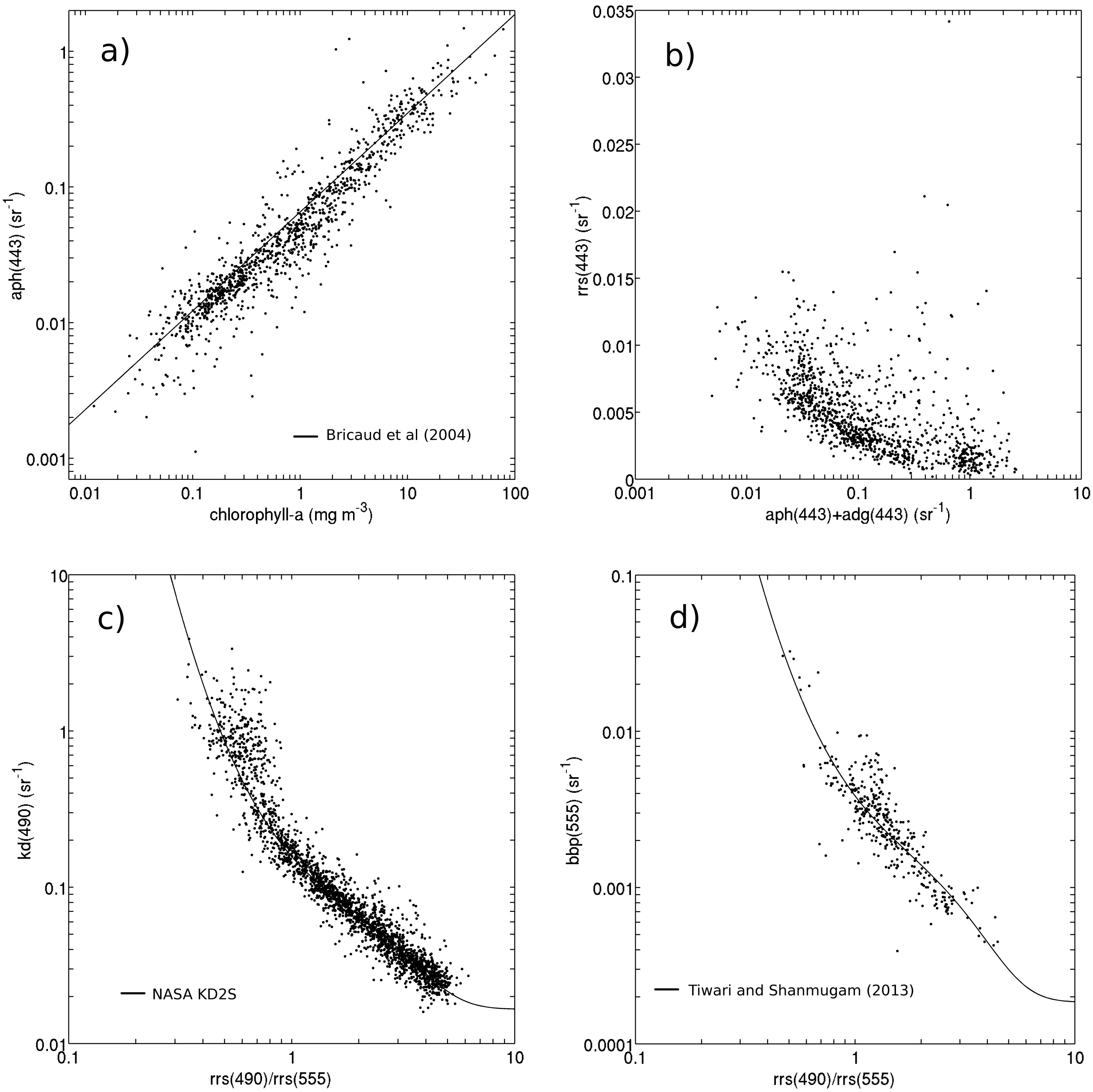

Figure 15. Examples of bio-optical relationships in the final merged table. (a) aph(443) versus chlorophyll-a. Total number of points (1,070) is divided between MERMAID (70), NOMAD (991) and SeaBASS (9). For reference the solid line show

the regression from Bricaud et al. (2004). (b) [aph(443) + adg(443)] versus rrs(443). Total number of points (1,112) is divided between MERMAID (33) and NOMAD (1,079). (c) [rrs(490)/rrs(555)] versus kd(490). The total number of points (2,280) is divided between MERMAID (62), NOMAD (2,117) and SeaBASS (101). For reference the solid line show the NASA KD2S standard algorithm (http://oceancolor.gsfc.nasa.gov/cms/atbd/kd_490). (d) [rrs(490)/rrs(555)] versus bbp(555). The total number of points (357) is divided between MERMAID (33) and NOMAD (324). For reference the solid line show the relation proposed by Tiwari and Shanmugam (2013). A search window of 2 nm was used for (a) and (b), and a search window of 5 nm was used for (c) and (d) to include data at 560 nm when not available at 555 nm.