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Open Access Earth System Science Data Discussions

A global database of dissolved organic matter (DOM) measurements in coastal waters (CoastDOM v1)

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Abstract

The measurements of dissolved organic carbon (DOC), nitrogen (DON), and phosphorus (DOP) are used to characterize the dissolved organic matter (DOM) pool and are important components of biogeochemical cycling in the coastal ocean. Here, we present the first edition of a global database (CoastDOM v1; available at https://figshare.com/s/512289eb43c4f8e8eaef) compiling previously published and unpublished measurements of DOC, DON, and DOP collected in coastal waters. These data are complemented by hydrographic data such as temperature and salinity and, to the extent possible, other biogeochemical variables (e.g., Chlorophyll-*a*, inorganic nutrients) and the inorganic carbon system (e.g., dissolved inorganic carbon and total alkalinity). Overall, CoastDOM v1 includes observations from all continents however, most data were collected in the Northern Hemisphere, with a clear gap in coastal water DOM measurements from the Southern Hemisphere. The data included were collected from 1978 to 2022 and consist of 62339 data points for DOC, 20360 for DON and 13440 for DOP. The number of measurements decreases progressively in the sequence DOC > DON > DOP, reflecting both differences in the maturity of the analytical methods and the greater focus on carbon cycling by the aquatic science community. The global database shows that the average DOC concentration in coastal waters (average (standard deviation; SD): 182 (314) µmol C L^{-1}; median: 103 µmol C L^{-1}), is 13-fold greater than the average coastal DON concentrations (average (SD): 13.6 (30.4) µmol N L^{-1}; median: 8.0 µmol N L^{-1}), which was itself 39-fold greater than the average coastal DOP concentrations (average (SD): 0.34 ± 1.11 µmol P L^{-1}; median: 0.18 µmol P L^{-1}). This dataset will be useful to identify global spatial and temporal patterns in DOM and to facilitate reuse of DOC, DON and DOP data in studies aimed at better characterising local biogeochemical processes, closing nutrient budgets, estimating carbon, nitrogen and

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phosphorous pools, as well as identifying a baseline for modelling future changes in coastal waters.

Keywords: Dissolved organic matter, Dissolved organic carbon, Dissolved organic nitrogen, Dissolved organic phosphorus, Coastal waters, Global database.

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1. Introduction

Coastal waters are the most biogeochemical dynamic areas of the ocean, exhibiting the highest standing stocks, process rates and transport fluxes of carbon (C), nitrogen (N), and phosphorus (P) per unit area (Bauer et al., 2013; Mackenzie et al., 2011). In these areas, organic matter plays a critical role in numerous biogeochemical processes, serving as both a C, N and P reservoir and substrate (Carreira et al., 2021).

Organic matter found in the marine environment is commonly distinguished by its size; material retained on a filter with a pore size typically between 0.2 and 0.7 μm is classified as particulate organic matter (POM), whereas organic matter that passes through the filter is referred to as dissolved organic matter (DOM). This partitioning is operational but has implications for biogeochemical cycling: POM can be suspended in the water column or sink to the sediments controlled by its size, shape and density (Laurenceau-Cornec et al., 2015), whereas DOM is a solute that mostly remains in the water column. In most coastal waters, the DOM concentrations are greater than POM, with the POM fraction being less degraded and more bioavailable (Boudreau and Ruddick, 1991; Lønborg et al., 2018).

The DOM pool consists mainly of C (DOC), N (DON), and P (DOP) but it also includes other elements such as oxygen, sulphur and trace elements (Lønborg et al., 2020). In coastal waters, DOM originates from multiple sources. Internal, or autochthonous, sources include planktonic organisms (Lønborg et al., 2009; Carlson and Hansell, 2015), benthic microalgae, macrophytes, and sediment porewater (Burdige and Komada, 2014; Wada et al., 2008). On the other hand, DOM from external, or allochthonous, sources, has mainly terrestrial origins, including wetlands, river and surface runoff, groundwater discharges, and atmospheric deposition (Iavorivska et al., 2016; Raymond and Spencer, 2015; Taniguchi et al., 2019; Santos et al., 2021). The main sinks for DOM from the water column in coastal waters are: 1) bubble coagulation and abiotic flocculation (Kerner et al., 2003) or sorption to particles (Chin et al., 1998); 2) sunlight mediated photodegradation

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(Mopper et al., 2015); and 3) microbial degradation by mainly heterotrophic prokaryotes (Lønborg and Álvarez-Salgado, 2012).

Given the importance of DOM as a source of nutrients and for coastal biogeochemical cycling in general, numerous studies have measured the C, N and P content of the DOM pool over the last few decades (e.g., García-Martín et al., 2021; Cauwet, 2002; Osterholz et al., 2021). Most data, however, are often unavailable or stored in an inaccessible manner, making it difficult to e.g., analyse global spatial and temporal patterns effectively. A global open ocean DOM data compilation already exists, but it contains few coastal samples (< 200m) (Hansell et al., 2021). Hence, there is a clear need for a comprehensive global and integrated database of DOC, DON and DOP measurements for coastal waters. To address this need, we have prepared the first edition of a coastal DOM database (named CoastDOM v1), by compiling both previously reported as well as unpublished data. These data have been obtained from authors of the original studies or extracted directly from the original studies. In order to allow the DOM measurements to be interpreted across larger scales, and to better understand their relationship with local environmental conditions, we have included concurrently collected ancillary data (such as physical and/or chemical seawater properties) whenever available. The objective of this database is multifaceted. Firstly, we aimed to compile all available coastal DOM data into a single repository. Secondly, our intention was to make these data easily accessible to the research community and thirdly, we sought to achieve long-term consistency of the measurements, to enable data intercomparison, and establish a robust baseline for assessing, for example, the impacts of climate change and land use changes.

2. Methods

2.1. Data compilation

The measurements included in CoastDOM v1 were obtained either directly from authors of previously published studies, online databases, or scientific papers. An extensive search of published reports, Ph.D. theses, and peer-reviewed literature was performed to identify studies dealing with DOM in coastal waters. First, a formal search was performed using Google Scholar in January 2022 using the search terms “dissolved organic carbon”, “dissolved organic nitrogen”, and “dissolved organic phosphorus” in connection with “marine” or “ocean”, which yielded a total of 897 articles (after filtering the query by searching content in the title and abstract and excluding non-coastal articles). When data could not be obtained directly from the corresponding authors, relevant data were extracted. Further searches for relevant datasets were conducted using the reference lists of the identified scientific papers as well as databases and repositories to capture as many datasets as possible. Additionally, research groups that were invited to participate in this effort were also encouraged to submit unpublished data to CoastDOM v1.

2.2. Dissolved organic matter analysis

The DOC concentrations included in CoastDOM v1 were commonly measured using a total organic carbon (TOC) high temperature catalytic oxidation (HTCO) analyser (81% of samples). Some were measured by a combined wet chemical oxidation (WCO) step and/or UV digestion, after which the carbon dioxide generated was quantified (19% of samples). Similarly, concentrations of total dissolved nitrogen (TDN) were determined using either a nitric oxide chemiluminescence detector connected in series with the HTCO analyser used for DOC analyses (31% of the samples), or by employing a UV and/or chemical oxidation step (69%). In the latter approach, both organic and inorganic N compounds were oxidised to nitrate, which was subsequently quantified through a colorimetric method to determine the concentration of inorganic N (Valderrama, 1981;

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Álvarez-Salgado et al., 2023; Halewood et al., 2022; Foreman et al., 2019). The reported DON concentrations were calculated as the difference between TDN and dissolved inorganic nitrogen (DIN; sum of ammonium (NH_4^+) and nitrate/nitrite (NO_3^- + NO_2^-); DON = TDN - DIN) (Álvarez-Salgado et al., 2023). Analyses of total dissolved phosphorus (TDP) were determined by UV (4%) or wet chemical oxidation (66%), or a combination of these (30%), and subsequently were analysed for inorganic phosphorus by a colorimetric method (Álvarez-Salgado et al., 2023). The DOP concentrations were calculated as the difference between TDP and soluble reactive phosphorus (SRP: HPO_4^{2-}) (DOP = TDP - SRP) (Álvarez-Salgado et al., 2023).

3. Description of the dataset

The data compiled in CoastDOM v1 were collected, analysed and processed by different laboratories, however, all data included have undergone quality control measures, either by using reference samples or internal quality assurance procedures. While many of the included DOC and TDN data have been systematically compared against consensus reference material (CRM) mainly provided by the University of Miami's CRM program (Hansell, 2005), there is a limitation in CoastDOM v1 regarding the intercalibration across different measurement systems used for both DOP and DON determination. While the CRM could be used for DOC, DON and DOP measurements, this has not yet been attempted for DOP and measurement uncertainties increase in the sequence DOC > DON > DOP. Although some of the reported measurements have quantified the DOP recovery based on commercially available DOP compounds such as Adenosine triphosphate (ATP), it is not known if these were conducted systematically in all cases. Therefore, we strongly recommend undertaking further intercalibrations across laboratories for future measurements of TDP, as has been done for DOC and TDN

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measurements (e.g., Sharp et al., 2002). Since additional quality control is not possible in retrospect, we assessed the quality of CoastDOM v1 based on its internal consistency.

In CoastDOM v1, we defined "coastal water" as encompassing estuaries (salinity > 0.1) to the continental shelf break (water depth < 200 m). However, some locations, such as deep fjords which are close to the coast cannot be classed as coastal due to bathymetry (deeper than > 200 m). Therefore, we evaluated the inclusion of some datasets on a case-by-case basis. For inclusion in the database, each DOM measurement needed at a minimum to contain the following information (if reported in the original publication or otherwise available):

- Country where samples were collected
- Latitude of measurement (in decimal units)
- Longitude of measurement (in decimal units)
- Year of sampling
- Month of sampling
- Sampling day (when available)
- Depth (m) at which the discrete sample were collected
- Temperature (°C) of the sample
- Salinity of the sample
- Dissolved organic carbon (DOC) concentration (µmol L^{-1})
- Method used to measure DOC concentration
- DOC - QA flag: Quality flag for DOC measurement
- Dissolved organic nitrogen (DON) concentration (µmol L^{-1})
- Total dissolved nitrogen (TDN) concentration (µmol L^{-1})
- Method used to measure TDN concentration
- TDN - QA flag: Quality flag for TDN measurement
- Dissolved organic phosphorus (DOP) concentration (µmol L^{-1})

- Total dissolved phosphorus (TDP) concentration (µmol L^{-1})
- Method used to measure TDP concentration
- TDP - QA flag: Quality flag for TDP measurement
- Responsible person
- Originator institution
- Contact of data originator

It should be noted that in all entries, at least DOC, DON or DOP should have been measured. In addition, we also included other relevant data, when available, in the CoastDOM v1 dataset:

- Depth at the station where the sample was collected (Bottom depth, m).
- Total suspended solids (TSS) concentration (mg L^{-1})
- Chlorophyll-*a* (Chl *a*) concentration (µg L^{-1})
- Chl *a* - QA flag: Quality flag for chlorophyll-*a* measurement
- Sum of nitrate and nitrite (NO_3^-+NO_2^-) concentration (µmol L^{-1})
- NO_3^-+ NO_2^- - QA flag: Quality flag for NO_3^-+ NO_2^- measurement
- Ammonium (NH_4^+) concentration (µmol L^{-1})
- NH_4^+ - QA flag: Quality flag for NH_4^+ measurement
- Soluble reactive phosphorus (HPO_4^{2-}) concentration (µmol L^{-1})
- HPO_4^{2-} - QA flag: Quality flag for HPO_4^{2-} measurement
- Particulate organic carbon (POC) concentration (µmol L^{-1})
- Method used to measure POC concentration
- POC - QA flag: Quality flag for POC measurement
- Particulate nitrogen (PN) concentration (µmol L^{-1})
- Method used to measure PN concentration
- PN - QA flag: Quality flag for PN measurement
- Particulate phosphorus (PP) concentration (µmol L^{-1})

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- Method used to measure PP concentration
- PP - QA flag: Quality flag for PP measurement
- Dissolved inorganic carbon (DIC) concentration (µmol kg^{-1})
- DIC - QA flag: Quality flag for DIC measurement
- Total alkalinity (TA) concentration (µmol kg^{-1})
- TA - QA flag: Quality flag for TA measurement

Quality control of large datasets is crucial to ensure their reliability and usefulness. Thus, we have not included data that were deemed compromised, such as records that had not gone through quality control by the data originators. We also accepted a certain degree of measurement error since multiple groups have been involved in the collection, analysis, and/or compilation of the information. Some of these errors were corrected (e.g., when a value was placed in a wrong column, or clearly inaccurate locations were reallocated for consistency with the place of study), while others could not be rectified (e.g., values showing clear signs of contamination) and were consequently excluded from CoastDOM v1. It should also be noted that differences in analytical capabilities between laboratories and individual measurement campaigns likely caused additional uncertainty. Outliers, arising for example from contamination, were removed from the dataset. The data were moreover screened for zero values (i.e., concentrations below the detection limit or absence of data). In cases where concentrations were below the detection limit, the zero values were replaced with half the value of the limit-of-detection. To ensure the inclusion of only high-quality data, we only accepted entries with specific World Ocean Circulation Experiment (WOCE) quality codes: "2- Acceptable measurement" and "6- Mean of replicate measurements". In our quality control assessments, we carefully avoided overly strict criteria, known as "data grooming", which could potentially overlook genuine patterns and changes in the dataset that may be significant over longer temporal

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and/or wider spatial scales. Coastal waters are known to exhibit a wide range of environmental concentrations, influenced by factors such as seasonality and local anthropogenic activities. Consequently, these data points may encompass a wide concentration range.

3.1 Summary of dissolved organic carbon (DOC) observations

Measurements of DOC concentrations were conducted between 1978 to 2022, with a total of 62339 individual data points (Table 1). The DOC concentrations ranged from 17 to 30327 µmol C L^{-1} (average (Standard Deviation; SD): 182 (314) µmol C L^{-1}; median: 103 µmol C L^{-1}; Table 1). The majority (53%) of the concentrations fell within the range of 60 to 120 µmol C L^{-1} (Fig. 1). A large number of DOC observations (17%) ranged between 300 and 600 µmol C L^{-1}, which were predominantly collected in eutrophic and river-influenced coastal waters of the Northern Hemisphere, such as the Baltic Sea (Fig. 1). It was observed that 75% of the DOC concentrations were higher than 77 µmol C L^{-1}, while 25% of the measurements surpassed 228 µmol C L^{-1} (Table 1).

Coastal environments that experience minimal continental runoff, such as Palmer Station in Antarctica, typically exhibit low DOC concentrations. On the other hand, coastal waters heavily influenced by humic-rich terrigenous inputs, such as the Sarawak region in Malaysia, tended to have high DOC concentrations. In addition some extreme high DOC concentrations were measured in the Derwent River in Australia which is impacted by paper mill effluents. There has been a large increase in the number of DOC observations after 1992 (Fig. 2), and those measurements were from a wide range of locations. However, these observations were not evenly distributed, with the Southern Hemisphere being relatively under-sampled, especially in the African, South American and Antarctic continents (Fig. 2, 3).

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3.2. Summary of dissolved organic nitrogen (DON) observations

The DON measurements were collected between 1990 and 2021, with a total of 20357 data points (Table 1). Concentrations of DON ranged from < 0.1 to 2095.3 µmol N L^{-1} (average (SD): 13.6 (30.4) µmol N L^{-1}; median: 8.0 µmol N L^{-1}; Table 1), with the most common range (42%) for DON concentrations between 4 to 8 µmol N L^{-1} (Fig. 1). Overall 75% of DON concentrations were above 5.5 µmol N L^{-1}, while 25% were above 15.8 µmol N L^{-1} (Table 1).

The lowest DON concentrations were recorded in Young Sound, Greenland, which receives direct run-off from the Greenland Ice Sheet, whereas the highest concentrations were detected during a flood event in the Richmond River Estuary, Australia. Since 1995, there has been a large increase in the number of DON measurements conducted in coastal waters globally (Fig. 2); however, the majority of those measurements have been in the Northern Hemisphere, mostly in Europe and the United States (Fig. 2, 3).

3.3. Summary of dissolved organic phosphorus (DOP) observations

CoastDOM v1 includes a total of 13534 DOP measurements, collected between 1990 and 2021 (Table 1). Overall, DOP concentrations ranged from < 0.10 to 84.27 µmol P L^{-1} (average (SD): 0.34 (1.11) µmol P L^{-1}; median: 0.18 µmol P L^{-1}; Table 2). The majority (74%) of DOP concentrations were below 0.30 µmol P L^{-1} (Fig. 1). Analysis of the DOP dataset revealed that 75% of the concentrations were above 0.11 µmol P L^{-1}, while 25% were above 0.30 µmol P L^{-1} (Table 1).

The lowest DOP concentrations were measured off the Kimberley Coast in Australia, while the highest concentrations were found in the Vasse-Wonnerup Estuary in the South west region of Australia. Similarly to DOC and DON, most of the DOP measurements have been conducted from the 1990s onwards, with a predominant focus in the Northern Hemisphere, particularly in Europe and the United States (Fig. 2, 3).

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3.4. Summary of dissolved organic matter (DOM) observations

In CoastDOM v1 the number of measurements decreases progressively in the sequence DOC > DON > DOP, reflecting both differences in the maturity of the analytical methods and the greater focus on carbon cycling by the aquatic science community. In addition the average DOC concentration in coastal waters (182 (314) µmol C L^{-1}), was 13-fold greater than the average coastal DON concentrations 13.6 (30.4) µmol N L^{-1}), which was itself 39-fold greater than the average coastal DOP concentrations (0.34 (1.11) µmol P L^{-1}) (Table 1). Interestingly the coefficient of variation (C.V.) increased from DOC (173%) to DON (224%) and DOP (326%), which is related to that the % contribution of refractory organic material decreases in the same sequence (Table 1).

3.5. Potential use of the dataset

The use of the CoastDOM v1 dataset should be accompanied by the citation of this paper and the inclusion of the correct doi-reference. CoastDOM v1 will be available in full open access on the PANGEA homepage after acceptance of the manuscript, where it will be available as a *.csv file. The dataset includes a brief description of the metadata and methods employed, with emphasis on measurement techniques and data units. We chose the terminology most familiar to the ocean science community. It is important to note that all data included in CoastDOM v1, as well as this manuscript, are considered public domain; as such, a subset of this global dataset may also be present in previous data compilations (e.g., Hansell et al., 2021). The list of citations and links referenced in CoastDOM v1 also provide users with information as to how these data has been previously used in publications or databases.

3.6. Recommendations and conclusions

In CoastDOM v1, we have compiled available coastal DOM data in a single repository, making it freely available to the research community. This compilation has established a consistent global dataset, serving as a valuable information source to investigate a variety of environmental questions and to explore spatial and temporal trends. We suggest a set of recommendations for the future expansion of this global dataset. Firstly, our analysis highlights a spatial bias, with a concentration of sampling efforts and/or data availability predominantly concentrated in the Northern Hemisphere. The data gap in coastal DOM measurements in the Southern Hemisphere needs to be addressed to provide a more representative global understanding of the role of DOM in coastal water biogeochemistry. Additionally, increased sampling efforts especially in the African and South American continents are warranted due to the vulnerability of many coastal areas to climate change and intensifying human activities, which will undoubtedly impact DOM biogeochemistry. Further it is also worth noting that there is comparatively few data from coastal waters affected by river discharge into the tropics, e.g., Amazon, Indian and Indonesian rivers that together dominate freshwater inputs to the coastal ocean. Secondly, there is a need for more comprehensive temporal and spatial datasets to capture the variability of DOM levels in highly dynamic and productive coastal systems. Focused efforts should be made to resolve these temporal and spatial changes. Thirdly, it is also important to collect and report ancillary data, such as temperature, salinity, nutrient measurements, and particulate components, to provide context and better understand the underlying processes driving the observed DOM levels. Lastly, we strongly recommend that the DOM research community conducts regular inter-calibration exercises to establish standardised and interoperable methods, particularly for DON and DOP measurements. This will ensure the comparability and reliability of data across different studies and enhance our understanding of DON and DOP dynamics in coastal waters.

In light of ongoing global environmental changes, the mobilisation and open sharing of existing data of important biogeochemical variables, such as the DOM pool, are crucial for establishing baselines and determining global trends and changes in coastal waters. The aim is to publish an updated version of the database periodically to determine global trends of DOM levels in coastal waters, and we therefore encourage researchers to submit new data to the corresponding author. The CoastDOM v1 dataset was developed according to the FAIR principles regarding Findability, Accessibility, Interoperability and Reusability of data. Thus, CoastDOM v1 will serve as a reliable open-source information resource, enabling in-depth analyses and providing quality-controlled input data for large scale ecosystem models.

4. Data availability

The dataset is available for the review process at Figshare https://figshare.com/s/512289eb43c4f8e8eaef). The dataset is furthermore submitted to the PANGEA database and is currently waiting to be assigned a Doi number (Lønborg et al., 2023). The file will be available as a *.csv merged file and will be available in full open access in the PANGEA database after acceptance of the manuscript.

Competing interests

The authors declare no competing interests.

Author Contribution

C.L., C.C., and X.A.A-S started the initiative and finalised the data compilation. All co-authors contributed data. C.L. wrote the manuscript with input from all co-authors.

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Figure legends

Figure 1. Histograms showing the distribution of observations for **a**) dissolved organic carbon (DOC), **b**) nitrogen (DON) and **c**) phosphorus (DOP), within defined concentration ranges in the coastal ocean. Note that the concentration ranges are not uniform in all cases due to the large difference in concentration levels.

Figure 2. **a**) Cumulative number of observations for dissolved organic carbon (DOC), nitrogen (DON), and phosphorus (DOP). Number of observations shown as a function of **b**) latitude, and **c**) longitude, grouped into bins of 10° latitude or longitude.

Figure 3. Global distribution of observations included in CoastDOM v1 for **a**) dissolved organic carbon (DOC), **b**) nitrogen (DON), and **c**) phosphorus (DOP). The black dots on the map represent the reported data that are included in the CoastDOM v1 database. Histograms show the distribution of observations for DOC, DON and DOP within defined concentration ranges in the continents where measurements are available. Maps were created using the GIS shape file obtained from Laurelle et al. (2013)

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Table 1. Descriptive statistics for the dissolved organic carbon (DOC), dissolved organic nitrogen (DON), and dissolved organic phosphorus (DOP) measurements included in the CoastDOM v1 dataset. The minimum (Min), maximum (Max), average values (Avg.) and standard deviation (SD), coefficient of variation (CV %), median, 25th and 75th percentiles (perc.) and number of samples (N) for each variable are shown.

	DOC μ**mol C L**$^{-1}$	**DON** μ**mol N L**$^{-1}$	**DOP** μ**mol P L**$^{-1}$
Min	17	< 0.1	< 0.01
Max	30327	2095.3	84.27
Avg. (SD)	182 (314)	13.6 (30.4)	0.34 (1.11)
Median	103	8.0	0.18
CV %	173	224	326
25th perc.	77	5.5	0.11
75th perc.	228	15.8	0.30
N	62339	20357	13534

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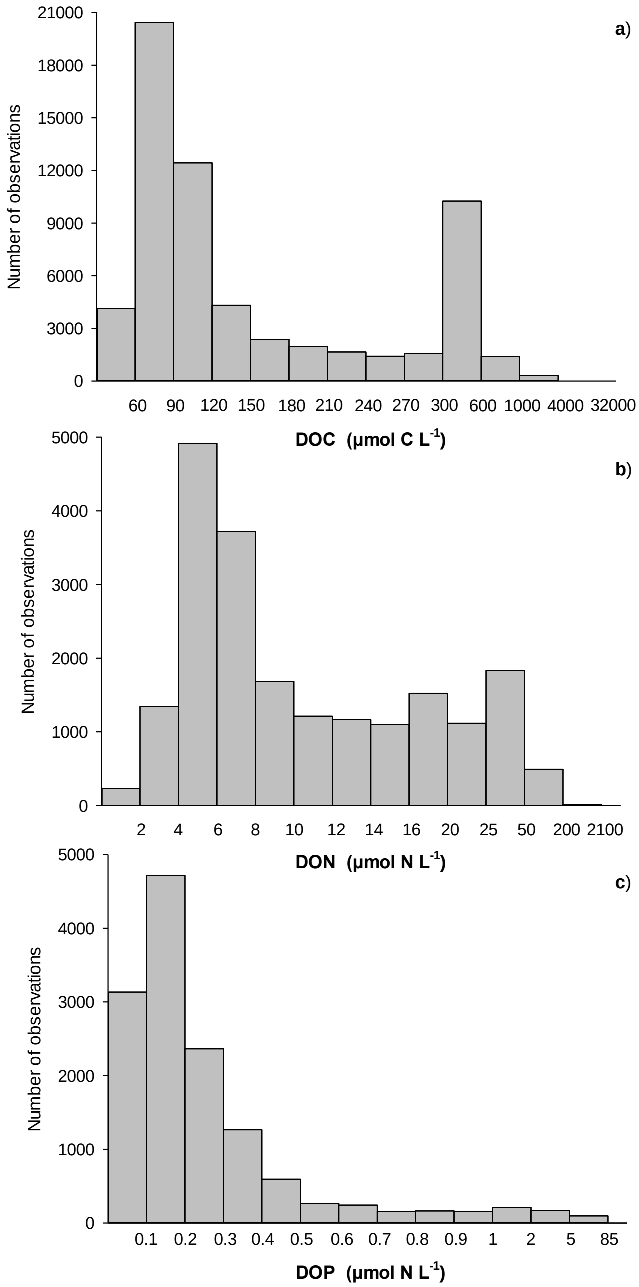

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707 **Figure 1.**

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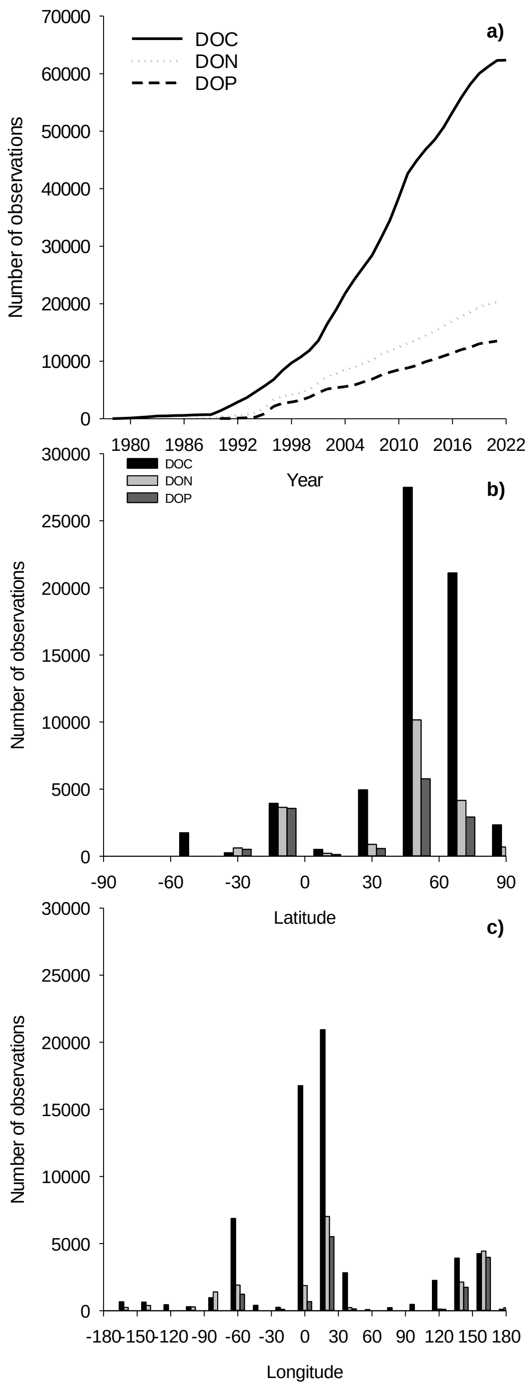

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709 **Figure 2.**

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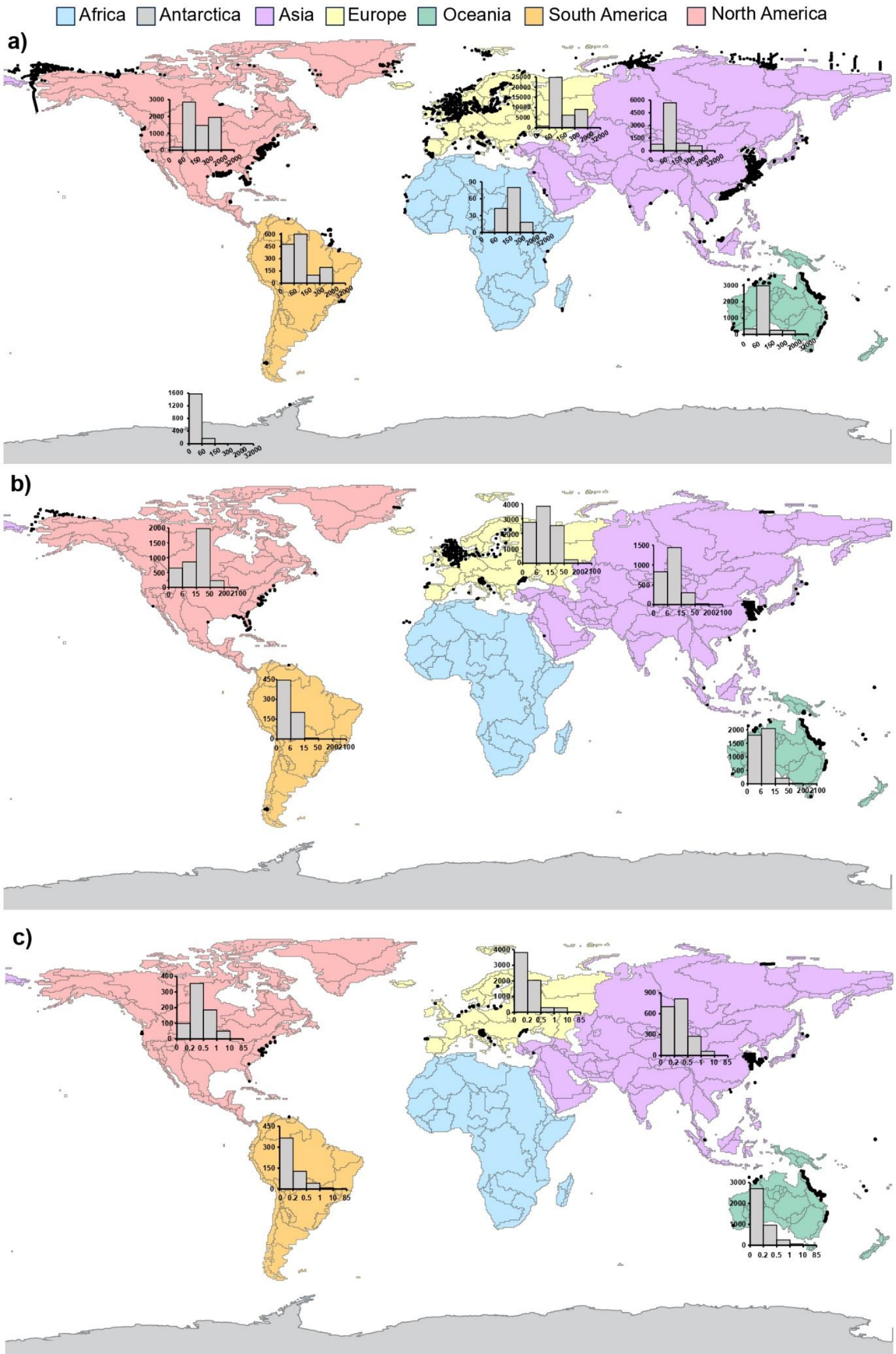

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711 **Figure 3.**