Dissolved DOC and TDN data from water samples collected at various sites around Puerto Rico during a Sargassum inundation event from May to June 2018

Website: https://www.bco-dmo.org/dataset/1010596
Data Type: Other Field Results
Version: 1
Version Date: 2026-10-22

Project
» Collaborative Research: Phlorotannins - An Important Source of Marine Chromophoric Dissolved Organic Matter? (Sargassum DOM)

Contributors	Affiliation	Role
Gonsior, Michael	Chesapeake Biological Laboratory (CBL)	Principal Investigator
Powers, Leanne	Chesapeake Biological Laboratory (CBL)	Scientist

Abstract
To compliment our work on Sargassum dissolved organic matter obtained during exudation experiments, we aimed to better understand the fate of Sargassum exudates and lysates in the environment. We sampled a Sargassum inundation event from 30 May to 6 June 2018 in Laguna Grande, Fajardo, Puerto Rico and other areas near Fajardo and Salinas, Puerto Rico. Laguna Grande is a 50-ha bioluminescent lagoon located in Las Cabezas de San Juan Nature Reserve in Fajardo, Puerto Rico. Sargassum had accumulated in the lagoon prior to sampling and dissolved oxygen (DO) was ~15 mg/L on May 30. On June 2, the lagoon was hypoxic (2.5 mg/L DO in the lagoon and 0.6 mg/L DO in the lagoon channel). From June 3 to 6, Sargassum had died (visible on seafloor) or was physically removed by humans and by June 6 the lagoon began to recover (4.5 mg/L DO). We also collected samples at a beach within the nature reserve and at Las Croabas, a beach adjacent to the lagoon channel where a dense accumulation of Sargassum was contained behind a barrier. Finally, we sampled a floating Sargassum mat in the coastal waters near Salinas, Puerto Rico. In all cases, we collected water samples underneath or at the mat's edge and at least ~15 m away from the mat. Filtered water samples were analyzed for dissolved organic carbon (DOC) and total dissolved nitrogen (TDN) concentrations directly. The remaining sample underwent solid phase extraction (SPE). Aliquots of these SPE methanolic extracts were dried and redissolved in ultrapure water for analysis of dissolved organic sulfur (DOS), -phosphorus (DOP), -bromine (DOBr), and -iodine (DOI) by inductively coupled plasma-mass spectrometry (ICP-MS). Additional aliquots of methanolic extracts dissolved in methanol were analyzed by Fourier transform-ion cyclotron mass spectrometry (FT-ICR MS).

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Coverage

Location: Coastal waters of Puerto Rico
Spatial Extent: **N**:18.5868 **E**:-65.5708 **S**:17.8476 **W**:-67.3709
Temporal Extent: 2018-05-30 - 2018-06-06

Methods & Sampling

Sample collection

Grab water samples (surface, ~0m) were collected dockside or by small boat in in 10-L low-density polyethylene cubitainers that had been pre-cleaned with 0.1 M NaOH for 24 h followed by several rinses of ultrapure Milli-Q water. Within 3 h of collection, samples for DOC and TDN analysis were 0.2-µm filtered through cellulose acetate filters into 40-mL combusted amber glass vials. Single samples for DOC/TDN were collected at each site, unless otherwise noted. The remaining samples were 0.7 µm-filtered through pre-combusted Whatman GF/F glass fiber filters into clean combusted 1-L bottles. SPE samples were collected in duplicate or triplicate. The 0.7 µm-filtered samples were then acidified to pH 2 using ultrapure concentrated HCl and underwent solid phase extraction (SPE). *Sargassum* exudates were generated by placing fragments of *Sargassum* in clear 500-mL Teflon bottles with seawater collected on the Atlantic shore with no visible *Sargassum*. Bottles were placed in a cooler with running water to maintain ambient temperature for 5 h. Seawater in bottles without *Sargassum* served as a control. After 5 h, exudates and the control were 0.7 µm-filtered as above and also underwent SPE.

Solid phase extraction (SPE)

We utilized 1 g Agilent Bond Elut PPL cartridges for SPE. Cartridges were activated with 10 mL ultrapure methanol and rinsed with 10 mL ultrapure 0.1% formic acid water prior to extraction. Samples were then loaded onto cartridges through clean Teflon tubing and extracted by gravity (final extraction volumes ranged from 0.4 to 1.2 L). After extraction, cartridges were rinsed with 30 mL 0.1% formic acid water and dried. Cartridges were then eluted in 10 mL ultrapure MeOH and these methanolic extracts were stored at -20 °C until ICP-MS and FT-ICR MS analysis.

ICP-MS

Dissolved organic compound (DOS, DOP, DOBr, DOI) analysis followed the methods described in Gonsior et al. (2024) (doi:10.1039/D3VA00361B) for DOS and DOP and in Powers et al. (2024) (doi: 10.1016/j.scitotenv.2023.169292) and Powers et al. (2026) (doi: 10.1029/2025GL119062) for dissolved organic bromine (DOBr) and dissolved organic iodine (DOI). Briefly, methanolic extract aliquots were dried under a gentle stream of nitrogen gas and redissolved in ultrapure water. Samples for DOBr and DOI analysis were also passed through silver cartridges prior to analysis to remove residual halides. DOS and DOP were analyzed by ICP-MS/MS using oxygen as the reaction gas and DOBr and DOI were analyzed by ICP-MS/MS with no gas in the Octopole Reaction System. Final concentrations were corrected for both extraction and dilution volumes. Reported values are the average and standard deviation of three replicate injections per sample.

Data Processing Description

Data processing details have not been detailed by the dataset author, please refer to the methods desription.

BCO-DMO Curation Notes

Curation Actions Performed on Data File

- Loaded PuertoRico_Sargassum_DOC_TDN.xlsx (XLSX, sheet 1, header row 1, formatting preserved) as table 1010596_v1_sargassum_inundation_event_doc_and_tdn_data; empty strings and “NA” were treated as missing values.
- Set column types: DOC, TDN, sdev_DOC, sdev_TDN, lat_dec, and long_dec as numbers; depth and n as integers; Sample_ID, Site, and location as strings; and Date as a date formatted %Y-%m-%d.
- Updated column metadata, including BCO-DMO descriptions, standard names, and supplied units, for DOC, TDN, sdev_DOC, sdev_TDN, Date, Sample_ID, Site, location, n, depth, lat_dec, and long_dec. Depth, lat_dec, and long_dec were flagged as primary parameters.
- Saved the final table as 1010596_v1_sargassum_inundation_event_doc_and_tdn_data.csv.

Problem Description

No problems or issues have been reported for this dataset by the dataset authors.

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Related Publications

Gonsior, M., Lahm, M., Powers, L., Chen, F., McCallister, S. L., Liang, D., Guinan, G., & Schmitt-Kopplin, P. (2024). Optical properties and molecular differences in dissolved organic matter at the Bermuda Atlantic and Hawai'i ALOHA time-series stations. Environmental Science: Advances, 3(5), 717–731. https://doi.org/10.1039/d3va00361b https://doi.org/10.1039/D3VA00361B
Methods

Powers, L. C., Schijf, J., Schmitt-Kopplin, P., & Gonsior, M. (2025). Halogenated Organic Compounds: A Massive Halogen Reservoir and an Intriguing Component of the Marine Dissolved Organic Matter Pool. Geophysical Research Letters, 53(1). Portico. https://doi.org/10.1029/2025gl119062 https://doi.org/10.1029/2025GL119062
Methods

Powers, L. C., Schmitt-Kopplin, P., & Gonsior, M. (2024). Evaluating the photochemical reactivity of disinfection byproducts formed during seawater desalination processes. Science of The Total Environment, 912, 169292. https://doi.org/10.1016/j.scitotenv.2023.169292
Methods

Tziotis, D., Hertkorn, N., & Schmitt-Kopplin, Ph. (2011). Kendrick-Analogous Network Visualisation of Ion Cyclotron Resonance Fourier Transform Mass Spectra: Improved Options for the Assignment of Elemental Compositions and the Classification of Organic Molecular Complexity. European Journal of Mass Spectrometry, 17(4), 415–421. https://doi.org/10.1255/ejms.1135
Methods

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Parameters

Parameter	Description	Units
Sample_ID	Unique identifier for the collected water or Sargassum exudate sample.	unitless
Site	Name of the sampling site where the water sample or exudate was collected.	unitless
location	Sampling position relative to the Sargassum mat: at or beneath the mat or mat edge, or approximately 15 m away from the mat.	unitless
Date	Date on which the sample was collected.	yyyy-mm-dd
n	Number of replicate measurements associated with the reported concentration and standard deviation.	count
lat_dec	Latitude of the sampling location in decimal degrees. Positive values indicate north latitude.	decimal degrees
long_dec	Longitude of the sampling location in decimal degrees. Negative values indicate west longitude.	decimal degrees
depth	Depth at which the water sample was collected, in meters. Samples were collected from the surface at approximately 0 m depth.	meters (m)
DOC	Dissolved organic carbon concentration measured in the filtered water sample.	mg C/L
sdev_DOC	Standard deviation of the replicate DOC measurements.	mg C/L
TDN	Total dissolved nitrogen (TDN) concentration measured in the filtered water sample.	mg N/L
sdev_TDN	Standard deviation of the replicate TDN measurements.	mg N/L

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Instruments

Dataset-specific Instrument Name	Agilent 8900 ICP-QQQ triple-quadrupole inductively coupled plasma mass spectrometer
Generic Instrument Name	Mass Spectrometer
Dataset-specific Description	We utilized 1 g Agilent Bond Elut PPL cartridges for SPE. Cartridges were activated with 10 mL ultrapure methanol and rinsed with 10 mL ultrapure 0.1% formic acid water prior to extraction. Samples were then loaded onto cartridges through clean Teflon tubing and extracted by gravity (final extraction volumes ranged from 0.4 to 1.2 L).
Generic Instrument Description	General term for instruments used to measure the mass-to-charge ratio of ions; generally used to find the composition of a sample by generating a mass spectrum representing the masses of sample components.

Dataset-specific Instrument Name	Bruker Solarix 12 Tesla FT-ICR mass spectrometer
Generic Instrument Name	Mass Spectrometer
Dataset-specific Description	Mass spectrometric analyses were undertaken at the Helmholtz Zentrum, Munich, Germany using a Bruker Solarix 12 Tesla Fourier transform ion cyclotron resonance mass spectrometer (FT-ICR MS) using negative electrospray ionization at -3600 V. The flow rate was 120 µL/h, 500 spectra were averaged. Pre-calibration was performed with arginine clusters and spectra were post-calibrated in the Bruker Data Analysis software using known DOM m/z ions across the m/z range of 200-700, with signal-to-noise set to 10.
Generic Instrument Description	General term for instruments used to measure the mass-to-charge ratio of ions; generally used to find the composition of a sample by generating a mass spectrum representing the masses of sample components.

Dataset-specific Instrument Name	Shimadzu Total Carbon Analyzer (TOC-Vcph)
Generic Instrument Name	Total Organic Carbon Analyzer
Dataset-specific Description	DOC and TDN concentrations were measured using a Shimadzu TOC-V.
Generic Instrument Description	A unit that accurately determines the carbon concentrations of organic compounds typically by detecting and measuring its combustion product (CO2). See description document at: http://bcodata.whoi.edu/LaurentianGreatLakes_Chemistry/bs116.pdf

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Project Information

Collaborative Research: Phlorotannins - An Important Source of Marine Chromophoric Dissolved Organic Matter? (Sargassum DOM)

Coverage: Mid-Atlantic Bight (July 2016), Sargasso Sea (July and September 2016), Coastal Bermuda (September/October 2016) and Coastal Puerto Rico (Laguna Grande, Fajardo; Las Croabas, Fajardo; Salinas; May/June 2018)

NSF Award Abstract:

Chromophoric dissolved organic matter (CDOM), the sunlight absorbing components in filtered water, is important in the study of marine and freshwater ecosystems as it can be used to trace the mixing of surface waters, as a proxy for carbon cycles, and other biogeochemical processes. Although its importance in ocean studies has been firmly established over the last several decades, sources and structural composition of CDOM within the oceans remains unclear and continues to be a subject of debate. Sargassum, a brown alga, is widely distributed in temperate and subtropical marine waters and may be important source of CDOM to the Sargasso Sea and Gulf of Mexico where Sargassum is abundant. This project will investigate the contribution of macro brown algae-derived compounds to the marine CDOM pool. Results from this study will have implications for the marine carbon cycle and satellite remote sensing of ocean color to assess mixing of surface water masses and biogeochemical processes. The project will provide educational opportunities for a postdoctoral scholar, summertime undergraduate internships (through a local NSF-sponsored Research Experiences for Undergraduates (REU) program), and workshop and research opportunities for local high schools students.

Sources of marine CDOM remain debatable and a comprehensive understanding of its origins, distribution and fate have been difficult. Marine CDOM, and in particular the "humic-like" component, have been suggested to originate from terrestrial sources, primarily lignins. However, recent evidence indicates that the exudation of phlorotannins produced by macro brown algae may contribute significantly to the marine CDOM pool. Phlorotannins, a class of polyphenols that are only found in, and continuously exuded by macro brown algae such as Sargassum, strongly absorb ultraviolet light and may have been underestimated in their contribution to the marine CDOM pool within certain geographic locales. Upon partial oxidation, light absorption by these specific compounds extends into longer wavelengths in the visible creating an absorption spectrum similar to that of lignin. These phlorotannins and their transformation products absorb light that might explain in part the "humic-like" signatures observed in open ocean environments. This study aims to characterize the optical properties and molecular composition of Sargassum-derived CDOM including its aerobic oxidation and photochemical behavior, as well as quantify Sargassum-derived CDOM to better estimate its possible contribution to the CDOM pool in the Sargasso Sea and Gulf of Mexico.

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1536888
NSF Division of Ocean Sciences (NSF OCE)	OCE-1536927

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