Ultrahigh resolution Mass Spectrometry data from a depth profile collected at 200 m depth intervals at the Bermuda Atlantic Time Series Station (BATS) in August 2019 and at the Hawaii Ocean Time Series station (HOTS) Aloha in July 2021

Website: https://www.bco-dmo.org/dataset/905077
Data Type: Other Field Results
Version: 1
Version Date: 2023-09-18

Project
» The fate of lysis products of picocyanobacteria contributes to marine humic-like chromophoric dissolved organic matter (Picocyanobacteria CDOM)

Contributors	Affiliation	Role
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Abstract
This data set contains ultrahigh resolution mass spectrometric data collected at BATS and HOTS at 200 m depth intervals in August 2019, and July 2021, respectively.

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Coverage

Spatial Extent: **N**:31.833333 **E**:-64.166667 **S**:22.75 **W**:-158
Temporal Extent: 2019-08 - 2021-07

Methods & Sampling

Water samples were collected using the ship's CTD profiler and 12 L Nisking bottles. 10 L water samples from each depth were then transferred into 5 gallon polycarbonate water bottles and extractrated. 10 L seawater samples were collected at 200 m depth intervals and then solid-phase extracted suing Agilent Bond Elut PPL cartridges (1 g, 6 ml). The organic matter was then eluted with 10 mL methanol. The methanolic extract was diluted 1:20 and directly infused into a 12 Tesla Bruker Solarix Fourier transform ion cyclotron resonance mass spectrometer. 500 scans were averaged and mass lists were calibrated at a mass accuracy of greater than 0.2 ppm.

Data Processing Description

Data were calibrated using known DOM signatures and a matrix was generated aligning all spectra. See Timko *et al.,* 2015 Reference for the calibration of FT-ICR MS data.

BATS depth 120m = deep chlorophyll maximum (DCM)
BATS depth 820m = oxygen minimum zone (OMZ)

BCO-DMO Curation Notes

* unpivot data: transform data from multiple intensity columns with location, depth and replicate in the header and changed it to one intensity column and added columns to capture the location, depth and replicate.
* added sampling date, latitude and longitude

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Data Files

File
905077_v1_massspec.csv (Comma Separated Values (.csv), 82.61 MB) MD5:858404187e9529766f5cd3fef5aac09f Primary datafile for dataset 905077

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Related Publications

Timko, S. A., Maydanov, A., Pittelli, S. L., Conte, M. H., Cooper, W. J., Koch, B. P., Schmitt-Kopplin, P., & Gonsior, M. (2015). Depth-dependent photodegradation of marine dissolved organic matter. Frontiers in Marine Science, 2. https://doi.org/10.3389/fmars.2015.00066
Methods

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Parameters

Parameter	Description	Units
Station_Location	Sampling station (HOT or BATS)	unitless
Latitude	Latitude sampling location, south is negative	decimal degrees
Longitude	Longitude sampling location, west is negative	decimal degrees
Date	Sampling date	unitless
Replicate	Replicate number	unitless
Depth	Sampling Depth	meters (m)
Mass	Mass to charge ratio (m/z)	unitless
Intensity	Ion intensity (arbitrary unit)	unitless

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Instruments

Dataset-specific Instrument Name	12 Tesla Bruker Solarix Fourier transform ion cyclotron resonance mass spectrometer
Generic Instrument Name	Fourier Transform Ion Cyclotron Resonance Mass Spectrometer
Generic Instrument Description	In Fourier Transform Ion Cyclotron Resonance Mass Spectrometry, the mass-to-charge ratio (m/z) of an ion is experimentally determined by measuring the frequency at which the ion processes in a magnetic field. These frequencies, which are typically in the 100 KHz to MHz regime, can be measured with modern electronics making it possible to determine the mass of an ion to within +/- 0.000005 amu or 5 ppm.

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Deployments

AE1920

Website	https://www.bco-dmo.org/deployment/905112
Platform	R/V Atlantic Explorer
Start Date	2019-08-08
End Date	2019-08-13

KM2110

Website	https://www.bco-dmo.org/deployment/905115
Platform	R/V Kilo Moana
Start Date	2021-07-06
End Date	2021-07-11

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Project Information

The fate of lysis products of picocyanobacteria contributes to marine humic-like chromophoric dissolved organic matter (Picocyanobacteria CDOM)

Coverage: Bermuda Atlantic Time Series Station (BATS) and station Aloha, Hawaii

NSF Award Abstract:
This study focuses on the sources and composition of colored dissolved organic matter (CDOM) in the ocean. CDOM is a part of water that absorbs sunlight. This material is important because it filters out harmful ultraviolet radiation. Scientists use it to track the movement of carbon and other important biological and chemical processes in the ocean. Organisms such as algae living in the open ocean have been shown to be sources of CDOM, but the chemical composition of these algal natural products remains to be discovered. Recent results from studying common algae show that viruses may break down algal cells and release material that looks like CDOM. This study will use new tools to find out if viruses and algae are creating this material and study its chemical makeup. This project will support two graduate students and provide summer internships for undergraduates through the NSF Research Experiences for Undergraduates (REU) program. The investigators will participate in a range of education and outreach activities.

The sources and structural nature of marine CDOM within the oceans remain unclear and continue to be a subject of debate. Marine in situ sources of CDOM have been suggested and some have been confirmed, but thus far none could explain the ubiquitous appearance of the so called "humic-like" CDOM component. Unique features of this component include its unusual exponential behavior in ultraviolet-visible (UV-Vis) absorbance with the absorbance extending well above 400 nm, and the large Stoke's shift in fluorescence spectroscopy. Picocyanobacteria are ubiquitous in the World's Oceans and make up 50 % of the autotrophic marine primary production. Preliminary results showed that the picocyanobacteria Synechococcus and Prochlorococcus release CDOM that matched the "humic-like" appearance of globally observed marine CDOM after virus-induced lysis. The main focus of this study is the characterization of the optical properties and molecular composition of viral-lysed DOM (VDOM) from different strains of Synechococcus and Prochlorococcus and additionally Trichodesmium which was shown in a previous study to also release CDOM. Associations between the chemical characterization information and metagenomics and transcriptomics data will be investigated for picocyanobacteria in the Pacific and Atlantic Oceans. This study includes long-term incubation experiments to determine the persistence of picocyanobacteria-derived CDOM as well as changes in microbial communities and processes (gene expression) that are related to the degradation of VDOM during the incubation period.

This award reflects NSF's statutory mission and has been deemed worthy of support through evaluation using the Foundation's intellectual merit and broader impacts review criteria.

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1829888

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