DOM analysis by liquid chromatography 21T fourier transform ion cyclotron resonance mass spectrometry with filtered seawater collected during a Bermuda Atlantic Time Series cruise AE1912 aboard R/V Atlantic Explorer in June of 2019

Website: https://www.bco-dmo.org/dataset/896754
Data Type: Cruise Results
Version: 1
Version Date: 2023-06-01

Project
» Collaborative Research: Determining the isotopic signature of iron released via ligand-mediated dissolution of atmospheric dust in the surface ocean (Dust Ligand Interactions)

Contributors	Affiliation	Role
Boiteau, Rene	Oregon State University (OSU)	Principal Investigator
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Abstract
This data set includes raw files obtained from the analysis of solid phase extracted marine dissolved organic matter (DOM) from the North Atlantic Subtropical Gyre by liquid chromatography coupled with ultra-high resolution mass spectrometry. Filtered seawater samples were collected in June 2019 during a Bermuda Atlantic Time Series cruise. DOM was isolated by solid phase extraction and analyzed by high pressure liquid chromatography with 21 Tesla Fourier Transform Ion Cyclotron Resonance Mass Spectrometry. The results provide insight into the molecular composition of DOM throughout the upper 1000m.

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Coverage

Spatial Extent: **N**:32.25 **E**:-64.166 **S**:31.833 **W**:-64.6
Temporal Extent: 2019-06-05 - 2019-06-11

Methods & Sampling

Location: Samples were collected in June 2019 on the R/V Atlantic Explorer from the Bermuda Atlantic Times Series (BATS) station and nearby stations at 31 50'N, 64 10'W from the upper 1000m.

Cruise or Deployment:

Samples were collected from the RV Atlantic Explorer (cruise V-1912 BATS/HYDRO/GRUNDLE) from June 5-11. Chief Scientist, Rod Johnson.

Methods & Sampling:
10 L samples were collected in June 2019 on the R/V Atlantic Explorer from the Bermuda Atlantic Times Series (BATS) station at 31 50'N, 64 10'W. Samples were pumped through polyethersulfone filters (Millipore Millex GP 0.2 µm, 25 mm) and then solid phase extracted onto 1 g polystyrene divinylbenzene resin columns (ENV, Agilent). Columns were preconditioned by sequentially rinsing with 6 mL LCMS grade methanol, 6 mL pH 2 ultrapure water (acidified with trace metal grade HCl), and 6 mL of ultrapure water prior to sample loading. A process blank sample was prepared by priming and rinsing an SPE column without sample loading. After sample loading, the columns were rinsed with 6 mL ultrapure water and stored frozen at –20 °C. Immediately prior to analysis, columns were thawed, rinsed again with 5mL ultrapure water, and eluted with 6mL of methanol. Samples were concentrated in a vacuum centrifuge to a volume below 0.5 mL until only residual water remained, and then samples were all brought up to a final volume of 0.8 mL with ultrapure water. An internal standard of cyanocobalamin was added to each sample (3 µM final concentration). Pooled quality control samples were prepared by combining 20 µL of each sample and were analyzed periodically throughout the sample batch in order to rule out significant drift in retention times or sensitivity.

Instruments:

Samples were analyzed by 21 Tesla Fourier Transform Ion Cyclotron Resonance Mass Spectrometer coupled to a microflow high pressure chromatography system (Ultimate 3000 RSLCnano, Thermo Scientific). The 21 T FT-ICR MS was designed and built in the Environmental Molecular Sciences Laboratory at the Pacific Northwest National Laboratory 26. The ESIMS was equipped with a heated electrospray ionization source set to a capillary voltage of 3200 V, sheath, auxiliary, and sweep gas flow rates of 15, 3, and 1 (arbitrary units), ion transfer tube temperature of 300°C, vaporizer temperature of 75°C. Mass spectra were collected with 1.5 second transients with a maximum ion accumulation time of 250 ms in positive ionization mode.

Data Processing Description

Thermo .RAW data was converted to a non-proprietary format (.mzML) using MSConvert version 3.0.18288 (ProteoWizard; https://proteowizard.sourceforge.io/; Chambers et al. (2012)) with 32-bit binary encoding precision. Data was centroided using the vendor filter algorithm.

BCO-DMO data manager notes:
* Files were packaged using 7z a -tzip and attached as "Data Files"
* no changes made to files themselves

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Data Files

File
MScovert .mzML format filename: MScovert_mzML_data.zip (Octet Stream, 2.41 GB) MD5:3f7fd687e4c914f6f5cc0378c323d083 This file bundled contains raw mass spectrometry data from LC-21T FT-ICR MS analysis of SPE DOM samples from BATS stations. These files contain data in .mzML format an open, XML-based format for mass spectrometer output files. Files are named with convention: "RMB_[yymmdd]_[sample identifier]_[depth]m.mzML" example filename: RMB_190828_BATS02_5m.mzML
Thermo .RAW format filename: Thermo_RAW_data.zip (Octet Stream, 11.67 GB) MD5:4b0f0267325315c2ad807b047795ffed This file bundled contains raw mass spectrometry data from LC-21T FT-ICR MS analysis of SPE DOM samples from BATS stations. These are raw data files (Thermo .RAW format) generated as outputs from 21T FT-ICR MS with no post-processing. Files are named with convention: "RMB_[yymmdd]_[sample identifier]_[depth]m.raw" example filename: RMB_190828_BATS02_5m.raw

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Supplemental Files

File
BATS sample list filename: BATS_samplelist.csv (Octet Stream, 4.22 KB) MD5:f315095be849b5cdcc8d203489f0ec71 List of LC-21T FT-ICR MS analyses. Parameter information [Column name, description, units]: File,Filename of Thermo .RAW format files contained in Thermo_RAW_data.zip., Sample type,"Sample type (e.g. pooled, sdmix) see methods.", Analysis order,Analysis order (numeric). , Sample number,Sample number, Niskin Bottle number,Niskin Bottle number, Cast,Cast, Sample collection date,Sample collection date in format %m/%d/%Y, Sample analysis date,Sample analysis date in format %m/%d/%Y, Volume (L),Volume,liters Depth (m),Depth,meters Station,Station, Longitude,Longitude,decimal degrees Latitude,Latitude, Cruise,Cruise, Sample Description,Sample Description,

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Related Publications

Chambers, M. C., Maclean, B., Burke, R., Amodei, D., Ruderman, D. L., Neumann, S., … Mallick, P. (2012). A cross-platform toolkit for mass spectrometry and proteomics. Nature Biotechnology, 30(10), 918–920. doi:10.1038/nbt.2377
Software

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Parameters

Parameters for this dataset have not yet been identified

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Instruments

Dataset-specific Instrument Name	Tesla Fourier Transform Ion Cyclotron Resonance Mass Spectrometer
Generic Instrument Name	Fourier Transform Ion Cyclotron Resonance Mass Spectrometer
Dataset-specific Description	Samples were analyzed by 21 Tesla Fourier Transform Ion Cyclotron Resonance Mass Spectrometer coupled to a microflow high pressure chromatography system (Ultimate 3000 RSLCnano, Thermo Scientific). The 21 T FT-ICR MS was designed and built in the Environmental Molecular Sciences Laboratory at the Pacific Northwest National Laboratory 26. The ESIMS was equipped with a heated electrospray ionization source set to a capillary voltage of 3200 V, sheath, auxiliary, and sweep gas flow rates of 15, 3, and 1 (arbitrary units), ion transfer tube temperature of 300°C, vaporizer temperature of 75°C. Mass spectra were collected with 1.5 second transients with a maximum ion accumulation time of 250 ms in positive ionization mode.
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.

Dataset-specific Instrument Name	Ultimate 3000 RSLCnano
Generic Instrument Name	Gas Chromatograph
Dataset-specific Description	Samples were analyzed by 21 Tesla Fourier Transform Ion Cyclotron Resonance Mass Spectrometer coupled to a microflow high pressure chromatography system (Ultimate 3000 RSLCnano, Thermo Scientific). The 21 T FT-ICR MS was designed and built in the Environmental Molecular Sciences Laboratory at the Pacific Northwest National Laboratory 26. The ESIMS was equipped with a heated electrospray ionization source set to a capillary voltage of 3200 V, sheath, auxiliary, and sweep gas flow rates of 15, 3, and 1 (arbitrary units), ion transfer tube temperature of 300°C, vaporizer temperature of 75°C. Mass spectra were collected with 1.5 second transients with a maximum ion accumulation time of 250 ms in positive ionization mode.
Generic Instrument Description	Instrument separating gases, volatile substances, or substances dissolved in a volatile solvent by transporting an inert gas through a column packed with a sorbent to a detector for assay. (from SeaDataNet, BODC)

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Deployments

AE1912

Website	https://www.bco-dmo.org/deployment/896800
Platform	R/V Atlantic Explorer
Start Date	2019-06-05
End Date	2019-06-10
Description	Project: BATS 10360, Hydro 61361

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Project Information

Collaborative Research: Determining the isotopic signature of iron released via ligand-mediated dissolution of atmospheric dust in the surface ocean (Dust Ligand Interactions)

Coverage: North Atlantic Subtropical Gyre

NSF abstract:
Iron (Fe) is a crucial nutrient for microbial growth in the oceans, impacting the carbon cycle and the climate system, but Fe does not dissolve readily in seawater and so its availability limits phytoplankton growth over much of the surface oceans. One of the most significant ways by which Fe reaches the surface oceans is through deposition of wind-blown dust; however, for this Fe to be available for biological growth, it must dissolve and be kept in solution bound to organic molecules. Despite this known importance, the mechanisms of dust dissolution and the identity of the organic molecules keeping Fe in solution remain poorly understood. This study will focus on using laboratory and field experiments to better understand how natural organic molecules present in seawater enhance the release of Fe from Saharan desert dust, the organic molecules produced by microbes in response to dust, the isotopic fractionation of Fe associated with dust dissolution, and ultimately the role of ligand-mediation dissolution in determining the role of dust in the marine Fe cycle. For outreach activities, the proposers would tutor refugee high school students from Africa/Asia in math and science to help them get integrated into the U.S. school system and discuss science with the public by participation in the St. Petersburg Science Festival. Three graduate students and undergraduate interns would be supported and trained as part of this project.

Scientists from the University of South Florida and Oregon State University will collect natural North Atlantic dust at the Tudor Hill Tower on Bermuda over a yearly cycle and characterize the weekly bulk and water-soluble Fe isotopic and elemental composition of the dust. Appropriate subsamples of this dust, representing both the Saharan and non-Saharan (anthropogenically-influenced) seasons will then be dissolved in seawater, with dissolution mediated by ligands with a range of Fe binding stability constants (natural ligands as well as defined marine siderophores). Incubations of dust will also be carried out with natural biological communities collected from the Gulf of Mexico and at the Bermuda Atlantic Time Series site in the North Atlantic. The investigators will characterize the amount and isotopic signature of the Fe released in each experiment, the microbial community response to dust in the incubations (DNA, cell counting and identification), and the ligands present in the natural organic matter used for experiments and produced in the incubations. Comparison of the abiotic and biological experiments will allow investigation of the magnitude of the biological effects on dust dissolution. The experiments will allow the investigators to provide a mechanistic understanding of factors that affect dust dissolution rates, especially the role of different specific organic ligands in enhancing and stabilizing the release of iron in the surface ocean, and the net signature of iron released. From this, the investigators will provide new constraints for the marine iron isotope cycle in the ocean, specifically testing the hypothesis that the net release of Fe from dust is isotopically heavy due to complexation with organic ligands, but that the size of this fractionation depends on the binding strength and presence of different ligands. The outcomes of this process study will provide a framework for models and interpretation of large scale field studies such as GEOTRACES, as well as enhancing the research community's ability to interpret aerosol and oceanic iron isotope data.

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-1829761

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