Sample information for metaproteomic samples taken from Station 2 from R/V Knorr KN210-04 in the Western Atlantic Ocean between Uruguay and Barbados from March 2013

Website: https://www.bco-dmo.org/dataset/875622
Data Type: Cruise Results
Version: 1
Version Date: 2022-06-13

Project
» Dissolved Organic Matter Composition in the Deep Atlantic Ocean (Deep Atlantic DOM)
» Deep Dissolved Organic Matter Multi-omics Analyses (DeepDom Multi-omics)

Programs
» Ocean Carbon and Biogeochemistry (OCB)
» Center for Chemical Currencies of a Microbial Planet (C-CoMP)
» Center for Chemical Currencies of a Microbial Planet (C-CoMP)

Contributors	Affiliation	Role
Saito, Mak A.	Woods Hole Oceanographic Institution (WHOI)	Principal Investigator
McIlvin, Matthew R.	Woods Hole Oceanographic Institution (WHOI)	Co-Principal Investigator
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Abstract
This dataset includes metadata from metaproteomic samples collected at Station 2 during the R/V Knorr Cruise KN210-04 in the Western Atlantic Ocean between Uruguay and Barbados in 2013. The accompanying total spectral counts for proteins and peptides from these samples are available on the PRoteomics IDEentifications Database (PRIDE) under Project PXD034035.

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Coverage

Spatial Extent: **Lat**:-38 **Lon**:-45
Temporal Extent: 2013-03-27 - 2013-03-29

Dataset Description

The dataset includes total spectral counts for proteins and peptides. Four files and a link to raw data at the domain repository are included:

1) Sample metadata file with station locations, depth, time of collection and sample IDs described by this BCO-

DMO page. (original file name: **DeepDOM_sample_metadata_for_OPP.csv)**

2) Raw mass spectral data files are available on PRIDE and ProteomeXchange:

ProteomeXchange title: Microbial Metaproteome from the Western Atlantic Ocean DeepDOM KN210-04 Expedition

ProteomeXchange accession: PXD034035

Project Webpage: http://www.ebi.ac.uk/pride/archive/projects/PXD034035

FTP Download: ftp://ftp.pride.ebi.ac.uk/pride/data/archive/2022/05/PXD034035

Methods & Sampling

Samples were collected by McLane Pump and filtered onto GFF and GF75 glass filters and frozen at -80C until analysis.

Filters were extracted using SDS detergent and tube gel purification followed by trypsin digestion alkylation and reduction. Analysis was conducted by 2D active modulation Orbitrap mass spectrometry as described in McIlvin and Saito 2021.

Data was collected with a Thermo Fusion Orbitrap mass spectrometer interfaced with a Dionex nano-HPLC configured with 2D active modulation chromatography using the methods of McIlvin and Saito 2021.

Data Processing Description

The raw mass spectra files were searched against SEQUEST high thread database within Proteome Discoverer software (v2.4). Processed files were then loaded into Proteome Software (Scaffold v5) and filtered to False Discovery rates less than 1% using Percolator. Protein and Peptide reports as well as discovered proteins fasta files will be generated. The files will be modified slightly to map to the Ocean Protein Portal data model for submission to BCO-DMO.

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Data Files

File
deepdom_sample_metadata_for_opp.csv (Comma Separated Values (.csv), 2.83 KB) MD5:97e4e94d3b8bae216b75c5e3f5dc4e06 Primary data file for dataset ID 875622.

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Related Publications

McIlvin, M. R., & Saito, M. A. (2021). Online Nanoflow Two-Dimension Comprehensive Active Modulation Reversed Phase–Reversed Phase Liquid Chromatography High-Resolution Mass Spectrometry for Metaproteomics of Environmental and Microbiome Samples. Journal of Proteome Research, 20(9), 4589–4597. doi:10.1021/acs.jproteome.1c00588
Methods

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Related Datasets

IsSupplementTo

Saito, M. A., McIlvin, M. R. (in prep) Microbial Metaproteome from the Western Atlantic Ocean DeepDOM KN210-04 Expedition. Proteomics Identifications Database (PRIDE). URL: https://www.ebi.ac.uk/pride/archive/projects/PXD034035
http://www.ebi.ac.uk/pride/archive/projects/PXD034035

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Parameters

Parameter	Description	Units
sample_id	sample identifier	unitless
ms_ms_sample_name	additional sample identifier that includes date of analysis run, method (2D), total amount of protein injected, cruise name, station number, pump cast number, filter type, and sample depth	unitless
station_id	station identifier	unitless
depth_m	Sample depth	meters
latitude_dd	latitude of sampling location with positive values indicating North	decimal degrees
longitude_dd	longitude of sampling location with positive values indicating West	decimal degrees
date_ISO	date of sample collection in ISO format	unitless
time_h_m_s	time of sample collection	unitless
minimum_filter_size_microns	minimum filter sized used reported in microns	microns
maximum_filter_size_microns	maximum filter sized used reported in microns	microns
cruise_id	cruise identifier	unitless
event_number	event identification number which includes sampling date in year-month-day format. This ID corresponds to the DeepDOM event log 'event' parameter.	unitless
ISO_DateTime_UTC	ISO standardized time and date of sampling.	unitless

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Instruments

Dataset-specific Instrument Name	nano-HPLC
Generic Instrument Name	High-Performance Liquid Chromatograph
Dataset-specific Description	Nano-HPLC configured with 2D active modulation chromatography.
Generic Instrument Description	A High-performance liquid chromatograph (HPLC) is a type of liquid chromatography used to separate compounds that are dissolved in solution. HPLC instruments consist of a reservoir of the mobile phase, a pump, an injector, a separation column, and a detector. Compounds are separated by high pressure pumping of the sample mixture onto a column packed with microspheres coated with the stationary phase. The different components in the mixture pass through the column at different rates due to differences in their partitioning behavior between the mobile liquid phase and the stationary phase.

Dataset-specific Instrument Name	Thermo Fusion Orbitrap mass spectrometer
Generic Instrument Name	Thermal Ionization Mass Spectrometer
Dataset-specific Description	Thermo Fusion Orbitrap mass spectrometer interfaced with a Dionex nano-HPLC configured with 2D active modulation chromatography.
Generic Instrument Description	A Thermal Ionization Mass Spectrometer (TIMS) is an instrument that measures isotopic ratios after electrical excitation of a sample causes ionization of the isotopes.

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Deployments

KN210-04

Website	https://www.bco-dmo.org/deployment/59057
Platform	R/V Knorr
Start Date	2013-03-25
End Date	2013-05-09
Description	Western Atlantic cruise started at Montevideo, Uruguay and ended at Bridgetown, Barbados. Science Objectives: 1. Characterize deep ocean dissolved organic matter in water masses of western Atlantic Ocean. 2. Characterize microbial community at selected stations and at selected depths. 3. Characterize metabolic capabilities of surface, mesopelagic and bathypelagic microbial consortia vis-a-vis the degradation of organic matter from each zone. 4. Examine metabolic and phylogenetic links between microbes in different marine zones (surface, meso-pelagic and bathypelagic depths). Science Activities: 1. Collection of discrete water samples by Niskin-bottles. 2. Collection of microbial communities from these water samples, by in-situ pumping, or by net-traps and net-tows. 3. Incubation experiments in lab and on deck. 4. Underway mass spectrometry and flow cytometry, from seawater intake. More information is available from the WHOI Cruise Planning Synopsis. Additional cruise information and original data are available from the NSF R2R Data Catalog.

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Project Information

Dissolved Organic Matter Composition in the Deep Atlantic Ocean (Deep Atlantic DOM)

Coverage: Western Atlantic Ocean

Transformations of dissolved organic matter (DOM) in the deep ocean have profound impacts on the global carbon cycle due to the sequestration of carbon dioxide (CO2) away from the atmosphere. Although research has been conducted on the high molecular weight component of this material, the same cannot be said for low molecular weight DOM because the needed analytical techniques have not been available to determine its composition and reactivity.

In recent years, a research team at Woods Hole Oceanographic Institution has acquired the necessary analytical capability. As such, in this project, they will carry out the first systematic survey of deep ocean DOM in the western Atlantic Ocean to characterize the low molecular weight fraction of DOM in southward flowing North Atlantic Deep Water (NADW), northward flowing Antarctic Bottom Water (AABW), and Antarctic Intermediate Water (AAIW). Using ultrahigh resolution mass spectrometry and multi-stage fragmentation coupled to liquid chromatography, the scientists will determine the spatial variability in the composition of DOM along the flow path of the water masses, as well as assess the source water, transport, and surface processes that contribute to temporal changes in DOM composition. These results will be augmented with structural elucidation and quantitative assays of unique marker compounds for each water mass. Results will provide important insights into the biogeochemical reactions that govern DOM dynamics in the deep ocean.

Deep Dissolved Organic Matter Multi-omics Analyses (DeepDom Multi-omics)

This project hosts additional dataset contributions to the Dissolved Organic Matter Composition in the Deep Atlantic Ocean Project (BCO-DMO Project 2204) that have been generated by the Center for Chemical Currencies of a Microbial Planet. This project will be focused on integrating data that has been collected using a variety of oceanographic sampling and 'omics techniques, including metabolomics and proteomics.

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Program Information

Ocean Carbon and Biogeochemistry (OCB)

Website: http://us-ocb.org/

Coverage: Global

The Ocean Carbon and Biogeochemistry (OCB) program focuses on the ocean's role as a component of the global Earth system, bringing together research in geochemistry, ocean physics, and ecology that inform on and advance our understanding of ocean biogeochemistry. The overall program goals are to promote, plan, and coordinate collaborative, multidisciplinary research opportunities within the U.S. research community and with international partners. Important OCB-related activities currently include: the Ocean Carbon and Climate Change (OCCC) and the North American Carbon Program (NACP); U.S. contributions to IMBER, SOLAS, CARBOOCEAN; and numerous U.S. single-investigator and medium-size research projects funded by U.S. federal agencies including NASA, NOAA, and NSF.

The scientific mission of OCB is to study the evolving role of the ocean in the global carbon cycle, in the face of environmental variability and change through studies of marine biogeochemical cycles and associated ecosystems.

The overarching OCB science themes include improved understanding and prediction of: 1) oceanic uptake and release of atmospheric CO2 and other greenhouse gases and 2) environmental sensitivities of biogeochemical

cycles, marine ecosystems, and interactions between the two.

The OCB Research Priorities (updated January 2012) include: ocean acidification; terrestrial/coastal carbon fluxes and exchanges; climate sensitivities of and change in ecosystem structure and associated impacts on biogeochemical cycles; mesopelagic ecological and biogeochemical interactions; benthic-pelagic feedbacks on biogeochemical cycles; ocean carbon uptake and storage; and expanding low-oxygen conditions in the coastal and open oceans.

Center for Chemical Currencies of a Microbial Planet (C-CoMP)

Website: https://ccomp-stc.org/

Coverage: North Atlantic, BATS, global/other

Functions carried out by microscopic inhabitants of the surface ocean affect every aspect of life on our planet, regardless of distance from the coast. Ocean phytoplankton are responsible for half of the photosynthesis on Earth, the first step in a complex system that annually withdraws 50 billion metric tons of carbon from the atmosphere to sustain their growth. Of this, 25 billion metric tons participate in a rapid cycle in which biologically reactive material is released into seawater and converted back into carbon dioxide by marine bacteria within hours to days. The chemical-microbe network at the heart of this fast cycle remains poorly constrained; consequently, its primary currencies and controls remain elusive; its sensitivities to changing ocean conditions are unknown; and its responses to future climate scenarios are not predictable. The Center for Chemical Currencies of a Microbial Planet (C-CoMP) integrates research, education and knowledge transfer activities to develop a mechanistic understanding of surface ocean carbon flux within the context of a changing ocean and through increased participation in ocean sciences. C-CoMP supports science teams that merge biology, chemistry, modeling, and informatics to close long-standing knowledge gaps in the identities and dynamics of organic molecules that serve as the currencies of elemental transfer between the ocean and atmosphere. C-CoMP fosters education, outreach, and knowledge transfer activities that engage students of all ages, broaden participation in the next generation of ocean scientists, and extend novel open-science approaches into complementary academic and industrial communities. The Center framework is critical to this mission, uniquely facilitating an open exchange of experimental and computational science, methodological and conceptual challenges, and collaborations that establish integrated science and education partnerships. With expanded participation in ocean science research and ocean literacy across the US society, the next generation of ocean scientists will better reflect the diverse US population.

Climate-carbon feedbacks on the marine carbon reservoir are major uncertainties for future climate projections, and the trajectory and rate of ocean changes depend directly on microbial responses to temperature increases, ocean acidification, and other perturbations driven by climate change. C-CoMP research closes an urgent knowledge gap in the mechanisms driving carbon flow between ocean and atmosphere, with global implications for predictive climate models. The Center supports interdisciplinary science teams following open and reproducible science practices to address: (1) the chemical currencies of surface ocean carbon flux; (2) the structure and regulation of the chemical-microbe network that mediates this flux; and (3) sensitivity of the network and its feedbacks on climate. C-CoMP leverages emerging tools and technologies to tackle critical challenges in these themes, in synergy with existing ocean programs and consistent with NSF’s Big Ideas. C-CoMP education and outreach activities seek to overcome barriers to ocean literacy and diversify participation in ocean research. The Center is developing (1) initiatives to expand ocean literacy in K-12 and the broader public, (2) ocean sciences undergraduate curricula and research opportunities that provide multiple entry points into research experiences, (3) post-baccalaureate programs to transition undergraduates into graduate education and careers in ocean science, and (4) interdisciplinary graduate student and postdoctoral programs that prepare the next generation of ocean scientists. The C-CoMP team includes education faculty who evaluate the impacts of education and outreach activities and export successful STEM initiatives to the education community. C-CoMP is revolutionizing the technologies for studying chemical transformations in microbial systems to build understanding of the outsized impact of microbes on elemental cycles. Open science, cross-disciplinary collaborations, community engagement, and inclusive practices foster strategic advances in critical science problems and STEM initiatives. C-CoMP science, education, and knowledge-transfer themes are efficiently addressed through a sustained network of scientists addressing critical research challenges while broadening the workforce that will tackle multi-disciplinary problems with academic, industrial and policy partners.

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.

The Program's Data Management Plan (DMP) is available as a PDF document.

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Coverage: North Atlantic, BATS, global/other

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-2019589

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