Targeted particulate metabolite abundances from R/V Knorr cruise KN210-04 in the Western Atlantic Ocean between Uruguay and Barbados from March to May 2013 (Deep Atlantic DOM project)

Website: https://www.bco-dmo.org/dataset/700038
Data Type: Cruise Results
Version:
Version Date: 2017-05-16

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

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

Contributors	Affiliation	Role
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Coverage

Spatial Extent: **N**:9.70268 **E**:-27.50038 **S**:-38.0026 **W**:-55.29942

Dataset Description

This dataset contains particulate metabolite abundances from seawater samples collected during the R/V Knorr cruise KN210-04 between 29 Mar 2013 and 06 May 2013 along the eastern coast of South America.

See related dataset:
Targeted metabolite abundances: dissolved

Sample depth, lat, lon, station, time, and cast are from CTD profiles are also included in this dataset. For more information about the data from CTDs refer to the following datasets:
CTD
event log

Some of these data will be published in the following publication (Kujawinski et al., 2017)

Methods & Sampling

Water samples were filtered through a ~0.7 um GF/F filter (Whatman) and an omnipore PTFE 0.2 um filter (Millipore). Filters were kept frozen at -80C until extraction. Samples were extracted in the laboratory according to protocols described in Kido Soule et al., 2015.

A Phenomenex C18 reversed phase column (Synergi Fusion, 2.1 x 150 mm, 4 um) coupled via a heated ESI source to a triple quadrupole mass spectrometer (Thermo Scientific TSQ Vantage) was used to measure metabolites (Kido Soule et al., 2015).

Data Processing Description

Peaks were detected and integrated using MAVEN (Melamud et al., 2010). Metabolites were quantified using calibration curves and MQ blanks were subtracted. For limits of detection please refer to Johnson et al., 2017.

BCO-DMO Data Manager Processing Notes:
* added a conventional header with dataset name, PI name, version date
* modified parameter names to conform with BCO-DMO naming conventions
* blank values replaced with no data value 'nd'
* changed micro (u) symbol to u in the data.
* lat/lon rounded to 5 decimal places
* time 0 padded if less than 4 numbers (731 -> 0731)
* added ISO_DateTime_UTC timestamp

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Data Files

File
metabolites_particulate.csv (Comma Separated Values (.csv), 42.17 KB) MD5:025dc0a078bac27d9c648541ac7eb451 Primary data file for dataset ID 700038

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Related Publications

Johnson, W. M., Kido Soule, M. C., & Kujawinski, E. B. (2017). Extraction efficiency and quantification of dissolved metabolites in targeted marine metabolomics. Limnology and Oceanography: Methods, 15(4), 417–428. doi:10.1002/lom3.10181
Methods

Kido Soule, M. C., Longnecker, K., Johnson, W. M., & Kujawinski, E. B. (2015). Environmental metabolomics: Analytical strategies. Marine Chemistry, 177, 374–387. doi:10.1016/j.marchem.2015.06.029
Methods

Kujawinski, E. B., Longnecker, K., Alexander, H., Dyhrman, S. T., Fiore, C. L., Haley, S. T., & Johnson, W. M. (2017). Phosphorus availability regulates intracellular nucleotides in marine eukaryotic phytoplankton. Limnology and Oceanography Letters, 2(4), 119–129. doi:10.1002/lol2.10043
Results

Melamud, E., Vastag, L., & Rabinowitz, J. D. (2010). Metabolomic Analysis and Visualization Engine for LC−MS Data. Analytical Chemistry, 82(23), 9818–9826. doi:10.1021/ac1021166
Software

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Parameters

Parameter	Description	Units
cast	cast number	unitless
station	station identifier	unitless
date_start_utc	date (UTC) in format yyyymmdd	unitless
time_start_utc	time (UTC) in format HHMM	unitless
ISO_DateTime_UTC	ISO timestamp based on the ISO 8601:2004(E) standard in format YYYY-mm-ddTHH:MM:SS[.xx]Z (UTC)	unitless
event_start	The event number from the ELOG maintained during the cruise.	unitless
lat_start	Latitude at the time the event started (from the cruise event log)	decimal degrees
lon_start	Longitude at the time the event started (from the cruise event log); west is negative	decimal degrees
depth	Depth from CTD. (Orignally called depSM)	meters (m)
filter_type	filter type	unitless
DOXP	1-deoxy-D-xylulose-5-phosphate concentration	picomolar (pM)
DHBA	2,3-dihydroxybenzoic acid concentration	picomolar (pM)
DHPS	2,3-dihydroxypropane-1-sulfonate concentration	picomolar (pM)
MPA	3-mercaptopropionate concentration	picomolar (pM)
PABA	4-aminobenzoic acid concentration	picomolar (pM)
PHBA	4-hydroxybenzoic acid concentration	picomolar (pM)
AdoHcy	S-(5'-adenosyl)-L-homocysteine concentration	picomolar (pM)
MTA	5-methylthioadenosine concentration	picomolar (pM)
adenine	adenine concentration	picomolar (pM)
adenosine	adenosine concentration	picomolar (pM)
AMP	adenosine 5'-monophosphate concentration	picomolar (pM)
arginine	arginine concentration	picomolar (pM)
aspartic_acid	aspartic acid concentration	picomolar (pM)
betaine	betaine concentration	picomolar (pM)

biotin	biotin concentration	picomolar (pM)
caffeine	caffeine concentration	picomolar (pM)
chitobiose	chitobiose concentration	picomolar (pM)
ciliatine	ciliatine concentration	picomolar (pM)
citrulline	citrulline concentration	picomolar (pM)
vitamin_B12	cyanocobalamin concentration	picomolar (pM)
cytosine	cytosine concentration	picomolar (pM)
desthiobiotin	desthiobiotin concentration	picomolar (pM)
GlcN_6_P	D-glucosamine 6-phosphate concentration	picomolar (pM)
DHAP	dihydroxyacetone phosphate concentration	picomolar (pM)
DMSP	DMSP concentration	picomolar (pM)
R5P	D-ribose 5-phosphate concentration	picomolar (pM)
folic_acid	folic acid concentration	picomolar (pM)
fosfomycin	fosfomycin concentration	picomolar (pM)
fumaric_acid	fumaric acid concentration	picomolar (pM)
G6P	glucose 6-phosphate concentration	picomolar (pM)
glutamic_acid	glutamic acid concentration	picomolar (pM)
glutamine	glutamine concentration	picomolar (pM)
glyphosate	glyphosate concentration	picomolar (pM)
guanine	guanine concentration	picomolar (pM)
IAA	indole 3-acetic acid concentration	picomolar (pM)
IMP	inosine 5'-monophosphate concentration	picomolar (pM)
inosine	inosine concentration	picomolar (pM)
cysteine	cysteine concentration	picomolar (pM)
glutathione	glutathione concentration	picomolar (pM)

leucine	leucine concentration	picomolar (pM)
methionine	methionine concentration	picomolar (pM)
GlcNAc	N-acetylglucosamine concentration	picomolar (pM)
Ac_Glu_OH	N-acetylglutamic acid concentration	picomolar (pM)
ornithine	ornithine concentration	picomolar (pM)
orotic_acid	orotic acid concentration	picomolar (pM)
pantothenic_acid	pantothenic acid concentration	picomolar (pM)
phenylalanine	phenylalanine concentration	picomolar (pM)
proline	proline concentration	picomolar (pM)
pyridoxine	pyridoxine concentration	picomolar (pM)
riboflavin	riboflavin concentration	picomolar (pM)
sarcosine	sarcosine concentration	picomolar (pM)
GPAT	sn-glycerol 3-phosphate concentration	picomolar (pM)
taurine	taurine concentration	picomolar (pM)
threonine	threonine concentration	picomolar (pM)
thymidine	thymidine concentration	picomolar (pM)
tryptophan	tryptophan concentration	picomolar (pM)
uracil	uracil concentration	picomolar (pM)
UMP	uridine 5'-monophosphate concentration	picomolar (pM)
xanthine	xanthine concentration	picomolar (pM)

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Instruments

Dataset-specific Instrument Name	Thermo Scientific TSQ Vantage
Generic Instrument Name	Mass Spectrometer
Dataset-specific Description	Phenomenex C18 reversed phase column (Synergi Fusion, 2.1 x 150 mm, 4 um) coupled via a heated ESI source to a triple quadrupole mass spectrometer (Thermo Scientific TSQ Vantage) was used to measure metabolites
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.

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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.

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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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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1154320

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