Biogeochemical Measurements from Surface Waters at the North Shore of Mo'orea, French Polynesia

Website: https://www.bco-dmo.org/dataset/942884 Data Type: Other Field Results Version: 1 Version Date: 2024-11-05

Project

» <u>Collaborative Research: Characterizing microbial transformation of marine DOM at the molecular level using</u> <u>untargeted metabolomic</u> (Metabolomics on the Mo'orea Reef)

Contributors	Affiliation	Role
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Abstract

This data includes biogeochemical and microbial parameters collected during spatial surveys on a coral reef at Mo'orea's North Shore (French Polynesia). Sampling took place in September 2017, May 2019, and April 2022. In 2019 and 2022, samples were also collected across three midday Lagrangian transect deployments. following water flowing linearly from ocean-facing forereefs over a reef crest to backreef lagoons. A variety of methods were used including colorimetric detection of inorganic nutrients, high-temperature combustion/oxidation, or chemical oxidation for the analysis of dissolved organic carbon (DOC) and particulate organic carbon and nitrogen (POC and PON) concentrations, isotope ratio mass spectrometry for determining stable carbon and nitrogen isotopes of particulate organic matter (POM), scanning excitation-emissions fluorescence measurements of whole seawater to quantify fluorescent dissolved organic matter (fDOM), flow cytometry-based cell counts to quantify bacterial abundance, and liquid chromatography coupled to tandem mass spectrometry to identify individual chemical features within marine DOM. These data help to quantify how biogeochemical parameters change in this region of the reef as open ocean waters flow onto the reef, over the reef, and then mix with waters in the bay. This work helps us to better identify external nutrients to the reef and how reef organisms modify and cycle carbon, nitrogen, and phosphorus over the reef. The results may be of use to physical, chemical, and biological oceanographers who study tropical reef systems and could inform other studies in the region including those conducted as part of the Mo'orea Coral Reef (MCR) Long Term Ecology Research (LTER) program. The samples were collected, measured (for a subset as noted below), and analyzed primarily by members of Lihini Aluwihare's group.

Table of Contents

- <u>Coverage</u>
- Dataset Description
 - Methods & Sampling
 - BCO-DMO Processing Description
- <u>Related Publications</u>
- <u>Parameters</u>
- <u>Project Information</u>
- <u>Funding</u>

Coverage

Spatial Extent: N:-17.4459786 **E**:-149.805 **S**:-17.50584 **W**:-149.8529899 **Temporal Extent**: 2017-09-22 - 2022-04-12

Methods & Sampling

Sample Collection:

Surface water was sampled at Mo'orea's North Shore (French Polynesia) (-17.47722, -149.84258) mid-day aboard kayaks or small motor boats in September 2017, May 2019, and April 2022. At every station on the backreef, salinity and temperature were measured using a YSI Professional Plus (Yellow Springs Instruments). Seawater samples were collected directly into 5-liter (L) polycarbonate carboys from the surface waters approximately 30 centimeters (cm) below the seawater surface and immediately transported to the shore for further processing. One milliliter (mL) of whole seawater was collected by pipette and added to a cryovial with 16 microliters (µL) of 32% paraformaldehyde, mixed by inversion, and immediately frozen and stored at -40 degrees Celsius (°C) for subsequent flow cytometric analysis of plankton abundance. Subsequent samples were processed using a multi-channel peristaltic pump and acid-washed silicone tubing initially flushed with approximately 300 mL seawater sample. For microbial community composition analysis, 300 to 500 mL sample was filtered through 0.2-micrometer (µm) polyethersulfone filter cartridges (Sterivex, Millipore, UK) and frozen at -40°C. The sterivex filtrate was used to rinse bottles to collect samples for inorganic nutrients, which were frozen and stored at -40°C. For particulate organic matter samples, 3 to 4L of seawater samples were filtered through pre-combusted GF/F (25mm, Whatman) filters, folded into combusted aluminum foil, and frozen at -40°C. For DOC measurements, GF/F filtrate was used to triple sample-rinse borosilicate vials with Teflon septa caps before collecting 40 mL (for deployment 2 and 3 in duplicates). Additionally, 2 liters of filtrate were also collected in triple-rinsed polycarbonate bottles for solid-phase DOM extraction. In total, 3 to 5 liters of sample were filtered through this G/FF filter via peristaltic pumps using acid-cleaned silicone tubing for analysis of particulate organic matter (POM). The filters were folded in half, wrapped in aluminum foil, and promptly frozen and stored at -80°C until analysis. DOC and DOM samples were acidified to pH 2 using trace metal grade HCl. Duplicates of acidified 1L DOM samples were solid-phase extracted using the multichannel pump operating at a flow rate of 18 milliliters per minute (mL/min) onto Bond Elut PPL resin cartridges (200 milligrams (mg) bed mass, Agilent 2105005, USA), according to (Dittmar et al., 2008) and (Petras et al., 2017). After desalinating the resin with LC-MS grade water (Fisher Chemical, Belgium), the cartridges were dried using Ultra High Purity compressed N₂ gas and kept frozen at -40°C.

Biogeochemical Measurements:

The following inorganic nutrients were analyzed using a Seal AA3 Segmented Flow Injection Autoanalyzer at the University of Hawai'i SOEST Laboratory for Analytical Biogeochemistry: Nitrate+nitrite (N+N) and silicate concentrations (Grasshoff et al., 1983), ammonium (Kérouel and Aminot, 1997), phosphate (Murphy and Riley, 1962). Additionally, total dissolved nitrogen and total dissolved phosphorus were determined through separate injections, with UV and alkaline or acid persulfate in-line oxidation, respectively. DOC samples were analyzed using high-temperature platinum catalytic oxidation on a Shimadzu TOC-V at the University of Santa Barbara, according to (Carlson et al., 2010) for data collected in 2017 and 2019. Data collected in 2022 were analyzed at Scripps Institution of Oceanography according to https://ccelter.ucsd.edu/dissolved-organic-carbon-and-totalnitrogen/, Particulate organic carbon (POC) and nitrogen (PON) concentrations were determined via filter combustion after acid fumigation to remove particulate inorganic carbon, drving, weighing, and packing into tin capsules (https://ccelter.ucsd.edu/particulate-organic-carbon-and-nitrogen/). Samples from 2017 were analyzed for carbon and nitrogen concentrations and stable isotope composition (δ 13C and δ 15N) at the SIO Stable Isotope Facility on a Thermo Finnigan DeltaPlus Isotope-Ratio mass spectrometer interfaced with a Costech 4010 elemental combustion analyzer. Filters from 2019 were analyzed on an Exeter Analytical CE 440 Elemental Analyzer in the SOEST Analytical Laboratory (http://www.soest.hawaii.edu/S-LAB/). The analysis of fluorescent dissolved organic matter (fDOM) was conducted using a Horiba Agualog scanning fluorometer, according to the methodology outlined in (Nelson et al., 2015). Samples for bacterioplankton enumeration were thawed and 200 µL of each sample was stained with SYBR Green I stain for a final concentration of 1X. Bacterial cell counts were enumerated using an Attune Acoustic Focusing Cytometer (Applied Biosystems, Part No. 4445280ASR) as described in (Nelson et al., 2015).

BCO-DMO Processing Description

currently being processed

[table of contents | back to top]

Related Publications

Carlson, C. A., Hansell, D. A., Nelson, N. B., Siegel, D. A., Smethie, W. M., Khatiwala, S., Meyers, M. M., Halewood, E. (2010). Dissolved organic carbon export and subsequent remineralization in the mesopelagic and bathypelagic realms of the North Atlantic basin. Deep Sea Research Part II: Topical Studies in Oceanography, 57(16), 1433–1445. doi:<u>10.1016/j.dsr2.2010.02.013</u> *Methods*

Dittmar, T., Koch, B., Hertkorn, N., & Kattner, G. (2008). A simple and efficient method for the solid-phase extraction of dissolved organic matter (SPE-DOM) from seawater. Limnology and Oceanography: Methods, 6(6), 230–235. doi:<u>10.4319/lom.2008.6.230</u> *Methods*

Grasshoff, K., Kremling, K., and Ehrhardt, M. (1983). Methods of Seawater Analysis. Verlag Chemia, Florida *Methods*

Kérouel, R., & Aminot, A. (1997). Fluorometric determination of ammonia in sea and estuarine waters by direct segmented flow analysis. Marine Chemistry, 57(3–4), 265–275. https://doi.org/10.1016/s0304-4203(97)00040-6 https://doi.org/10.1016/S0304-4203(97)00040-6 https://doi.org/10.1016/S0304-4203(97)00040-6 https://doi.org/10.1016/S0304-4203(97)00040-6 https://doi.org/10.1016/S0304-4203(97)00040-6 https://doi.org/10.1016/S0304-4203(97)00040-6 https://doi.org/10.1016/S0304-4203(97)00040-6

Murphy, J., & Riley, J. P. (1962). A modified single solution method for the determination of phosphate in natural waters. Analytica Chimica Acta, 27, 31–36. doi:10.1016/s0003-2670(00)88444-5 https://doi.org/10.1016/S0003-2670(00)88444-5 *Methods*

Nelson, C. E., Donahue, M. J., Dulaiova, H., Goldberg, S. J., La Valle, F. F., Lubarsky, K., ... Thomas, F. I. M. (2015). Fluorescent dissolved organic matter as a multivariate biogeochemical tracer of submarine groundwater discharge in coral reef ecosystems. Marine Chemistry, 177, 232–243. doi:<u>10.1016/j.marchem.2015.06.026</u> *Methods*

Petras, D., Koester, I., Da Silva, R., Stephens, B. M., Haas, A. F., Nelson, C. E., Kelly, L. W., Aluwihare, L. I., & Dorrestein, P. C. (2017). High-Resolution Liquid Chromatography Tandem Mass Spectrometry Enables Large Scale Molecular Characterization of Dissolved Organic Matter. Frontiers in Marine Science, 4. https://doi.org/<u>10.3389/fmars.2017.00405</u> *Methods*

[table of contents | back to top]

Parameters

Parameter	Description	Units
Sample_ID	Sample ID	unitless
Experiment	Experiment ID	unitless
MassiveID	Identification number for mass spectrometry data deposited on MassIVE (<u>https://massive.ucsd.edu/</u>)	unitless
MS_Sample_ID_1	File name of mass spectrometry data (LC-MS/MS; format: .raw and .mzML) for duplicate 1	unitless
MS_Sample_ID_2	File name of mass spectrometry data (LC-MS/MS; format: .raw and .mzML) for duplicate 2	unitless
Year	4-digit year of sample collection	unitless

Lon	Longitude of sample collection	decimal degrees
Lat	Latitude of sample collection	decimal degrees
DateTime_local	Local date and time of sample collection	unitless
ISO_DateTime_UTC_1	Date and time (UTC) of sample collection in ISO 8601 format	unitless
ISO_DateTime_UTC_2	Date and time (UTC) of sample collection in ISO 8601 format	unitless
ContactTime	Time after deployment for Lagrangian sample taken on the backreef	minutes
DOC	Dissolved Organic Carbon concentration	micromoles per liter (umol/L)
Total_N	Total Nitrogen concentration	micromoles per liter (umol/L)
Total_P	Total Phosphorus concentration	micromoles per liter (umol/L)
Phosphate	Phosphate concentration	micromoles per liter (umol/L)
Silicate	Silicate concentration	micromoles per liter (umol/L)
N_plus_N	Nitrate + Nitrite concentration	micromoles per liter (umol/L)
Ammonia	Ammonia concentration in water sample	micromoles per liter (umol/L)
PON	Particulate Organic Nitrogen based on GF/F filter analysis	micrograms per liter (ug/L)
POC	Particulate Organic Carbon based on GF/F filter analysis	micrograms per liter (ug/L)
PON15	Stable nitrogen isotope ratio of Particulate Organic Nitrogen (? 15N)	per mil (‰)
POC13	Stable carbon isotope ratio of Particulate Organic Carbon (? 13C)	per mil (‰)
Salinity	Salinity	practicial salinity units (PSU)

Temperature	Water temperature	degrees Celsius
PicoEukaryotes	PicoEukaryotes cell concentration	cells per microliter (cells/uL)
Prochlorococcus	Prochlorococcus cell concentration	cells per microliter (cells/uL)
Synechococcus	Synechococcus cell concentration	cells per microliter (cells/uL)
Heterotrophs	Heterotrophic bacterioplankton concentration	cells per microliter (cells/uL)
M_C_ratio	Humic to Protein-like ratio	Raman Fluorescence Units of Water
BIX	Biological index	Raman Fluorescence Units of Water
HIX	Humification Index	Raman Fluorescence Units of Water
FI	Fluorescence Index	Raman Fluorescence Units of Water
Ultra_Violet_Humic_like	Ultra Violet Humic-like component	Raman Fluorescence Units of Water
Marine_Humic_like	Marine Humic-like component	Raman Fluorescence Units of Water
Visible_Humic_like	Visible Humic-like component	Raman Fluorescence Units of Water
Tryptophan_like	Tryptophan-like component	Raman Fluorescence Units of Water
Tyrosine_like	Tyrosine-like component	Raman Fluorescence Units of Water
Phenylalanine_like	Phenylalanine-like component	Raman Fluorescence Units of Water
Fulvic_Acid_like	Fulvic Acid-like component	Raman Fluorescence Units of Water
Optical_Brighteners	Optical Brighteners component	Raman Fluorescence Units of Water
Diesel_Band_II	Diesel Band II component	Raman Fluorescence Units of Water
Petroleum_like	Petroleum-like component	Raman Fluorescence Units of Water

Lignin_like	Lignin-like component	Raman Fluorescence Units of Water
PARAFAC1	PARAFAC component 1	Raman Fluorescence Units of Water
PARAFAC2	PARAFAC component 2	Raman Fluorescence Units of Water
PARAFAC3	PARAFAC component 3	Raman Fluorescence Units of Water
PARAFAC4	PARAFAC component 4	Raman Fluorescence Units of Water
PARAFAC5	PARAFAC component 5	Raman Fluorescence Units of Water
PARAFAC6	PARAFAC component 6	Raman Fluorescence Units of Water

[table of contents | back to top]

Project Information

Collaborative Research: Characterizing microbial transformation of marine DOM at the molecular level using untargeted metabolomic (Metabolomics on the Mo'orea Reef)

Coverage: Mo'orea coral reefs

NSF Award Abstract:

Dissolved organic matter is an important component of the global carbon cycle. Dissolved organic matter provides food and energy for microbes living in the ocean and influences microbial diversity. Microbes convert some dissolved organic matter to CO2 (respiration) whereas other forms of dissolved organic matter are altered by microbial processes and persist in the ocean. Thus, it is important to understand how microbes change dissolved organic matter composition and reactivity. This project will examine the chemical structure of dissolved organic matter to identify: 1) molecules that fulfill carbon demand (biomass produced minus losses from respiration) and 2) transformation processes that result from microbial activity. The project will combine lab experiments and field studies at the Moorea Coral Reef Long Term Ecological Research site. The project will support training for three graduate students in marine biogeochemistry. Undergraduate training is aimed at sustained mentoring of underrepresented minority (URM) students. Undergraduates will be recruited from existing programs at Minority Serving Institutions at San Diego State University and the University of Hawai'i at Mānoa. Undergraduates will participate in the Scripps Institution of Oceanography SURF Research Experiences for Undergraduates program, where they will conduct research in marine chemistry. The goal is to provide a mentoring approach that can successfully overcome roadblocks to URM engagement in STEM and increase retention of these students in marine science.

This work will combine field and lab studies using advanced molecular-level chemical characterization tools to explore how bacteria alter the composition and bioreactivity of organic compounds dissolved in seawater. Additionally, this project will develop informatics-based tools to identify a larger proportion of chemical structures in marine dissolved organic matter (DOM) than is currently possible using traditional approaches. The project will use tandem mass spectrometry and networking techniques to comprehensively classify organic compounds into molecular families and determine common chemical transformations. Then, using a well-developed field-based experimental ecosystem to produce diverse labile DOM pools the research team will track microbial transformation using expression of hydrolytic enzymes and measure selection for particular microbial taxa and metabolisms. This approach defines the reactivity of individual molecules and broader compound classes participating in carbon fluxes that underpin DOM-microbe interactions. Field surveys conducted within the Moorea Coral Reef Long Term Ecological Research program will explore methods to track

transformation of specific molecules in the environment and validate experimental observations of compound classes that appear to accumulate as semi-labile DOM. By integrating laboratory and field experiments and oceanographic surveys with the refinement of analytical tools for untargeted metabolomics, this project will characterize the fate of reactive DOM in the ocean.

[table of contents | back to top]

Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	<u>OCE-2023509</u>
NSF Division of Ocean Sciences (NSF OCE)	OCE-2023298
NSF Division of Ocean Sciences (NSF OCE)	<u>OCE-2023707</u>
NSF Division of Ocean Sciences (NSF OCE)	OCE-2118618

[table of contents | back to top]