Reef seawater biogeochemistry data from samples collected in the Jardines de la Reina reef-system, Cuba in November of 2017

Website: https://www.bco-dmo.org/dataset/908026
Data Type: Other Field Results
Version: 1
Version Date: 2023-10-26

Project
» Signature exometabolomes of Caribbean corals and influences on reef picoplankton (Coral Exometabolomes)
» RAPID/MRI: Acquisition of a Triple-Quad Mass Spectrometer for Quantitative Identification of Dispersants and Water-Soluble Oil in the Gulf of Mexico (RAPID Mass Spec for Dispersants)

Contributors	Affiliation	Role
Apprill, Amy	Woods Hole Oceanographic Institution (WHOI)	Principal Investigator
Kujawinski, Elizabeth	Woods Hole Oceanographic Institution (WHOI)	Co-Principal Investigator
Gray, Laura	Woods Hole Oceanographic Institution (WHOI)	Scientist, Contact
York, Amber D.	Woods Hole Oceanographic Institution (WHOI BCO-DMO)	BCO-DMO Data Manager

Abstract
Reef depth and reef surface seawater samples were collected from reefs in Jardines de la Reina and subjected to targeted and untargeted liquid chromatography mass spectrometry (LC-MS) methods in addition to a suite of biogeochemical measurements (inorganic and organic nutrient concentrations, microbial cell abundances, chlorophyll a concentrations, and physicochemical properties). Raw and .mzML data files from the LC-MS methods are located at MetaboLights database, using accession number MTBLS1820. The link is: https://www.ebi.ac.uk/metabolights/MTBLS1820/. These data were published in Weber et al. (2020).

Table of Contents

- Coverage
- Dataset Description
  - Methods & Sampling
  - Data Processing Description
  - BCO-DMO Curation Notes
- Data Files
- Related Publications
- Related Datasets
- Parameters
- Instruments
- Project Information
- Funding

Coverage

Spatial Extent: **N**:21.3033 **E**:-78.3811 **S**:20.5065 **W**:-79.5911
Temporal Extent: 2017-11-05 - 2017-11-20

Dataset Description

Funding Description:

Dalio Foundation (now ‘OceanX’) (awarded to Amy Apprill)
National Science Foundation (OCE-1736288) (awarded to Amy Apprill)

Mass spectrometry samples were analyzed at the WHOI FT-MS Users’ Facility using instruments funded by the National Science Foundation (grant OCE-1058448 awarded to Elizabeth B. Kujawinski and Melissa Kido Soule)

and the Simons Foundation (Award ID #509042, awarded to Elizabeth B. Kujawinski)

Methods & Sampling

Location: Jardines de la Reina reef system south of the island of Cuba; General location: 20.8333° N, 78.9167° W

Sampling and analytical procedures:

Reef seawater microbial biogeochemistry and extracellular metabolite compositions (see "Related Datasets" section) were surveyed at nine, shallow (6 – 14 m in depth) forereef sites during a cruise to Jardines de la Reina (JR), Cuba in November of 2017. Seawater was also collected from two surface 'off reef' sites (800 – 1600 m depth).
At each reef, CTD (YSI Exo Sonde, Xylem Inc., Yellow Springs, OH, USA) casts were completed to measure the physicochemical properties of the water column. Seawater samples were collected from surface and reef depth to enumerate the number of microbial cells (1 mL samples) and assess macronutrient concentrations (30 mL for inorganic macronutrients and 40 mL for organic carbon and total nitrogen samples) using a submersible groundwater pump. Seawater samples (4L) were collected from reef depth and off reef samples for chlorophyll and phaeophytin analysis.
Samples collected for total organic carbon and nitrogen analyses were acidified with 75 µL of concentrated phosphoric acid, capped, and stored at room temperature. Surface and reef depth seawater samples collected for analyses of inorganic macronutrient concentrations (30 mL) were immediately frozen. Seawater, collected for enumeration of *Prochlorococcus*, *Synechococcus*, picoeukaryotic cells, and unpigmented cells (heterotrophic bacteria and archaea) was fixed with paraformaldehyde (1% final volume), incubated at 4 °C in the dark for 30 minutes, frozen at -50 °C on the research vessel, and then stored at -80 °C prior to analysis.

Non-purgeable total organic carbon (TOC, unfiltered), dissolved organic carbon (DOC, 0.2 µm filtered), total nitrogen (TN, unfiltered), and total dissolved nitrogen (TDN, 0.2 µm filtered) concentrations were analyzed using a Shimadzu TOC-VCSH total organic carbon analyzer (Hansell & Carlson, 2001) with a TNM-1 module. Inorganic macronutrient (phosphate, nitrite + nitrate, nitrite, ammonium, silicate) concentrations were measured with a continuous segmented flow system (as used in Apprill & Rappé, 2011). Nitrite was subtracted from the nitrite + nitrate concentrations to obtain the nitrate concentrations. Concentrations of total organic nitrogen were obtained by subtracting the sum of the inorganic nitrogen species (nitrite + nitrate and ammonium) from the total nitrogen concentrations per sample. If the measured concentrations fell beneath the detection limits of the instrument (ammonium = 0.02 M, phosphate = 0.01 M, nitrite + nitrate = 0.07 M, nitrite = 0.01 M), these measurements were removed from the analysis.

A few erroneous data values related to bottle/sample misidentification were included in the publication Weber et al. (2020). The differences between values are minor. The original values in Weber et al. (2020) are listed below and the corrected values are included within the dataset published here.

Reef name: JR4B_surf
The value for PO4 was 0.18
The value for SI was 1.6
The value for NO2 was 0.04
The value for NH4 was 0.03
The value for TON was 2.83

Reef name: OR2_surf
The value for TN was 0.18
The value for TON was -0.012

Acetone (90%) was used to extract Chlorophyll a and phaeophytin and the optical density (OD) values were measured on a calibrated spectrophotometer using standard optics (Lambda 18, Perkin Elmer, Waltham, MA, USA). The concentration ratios of chlorophyll a to phaeophytin were calculated and incorporated into the analyses. To obtain cell counts, flow cytometry was conducted using a collinear analysis method and a UV wavelength of 488 nm on an Altra flow cytometer at the University of Hawaii. Each sample was divided so that pigmented, fluorescent cells and unpigmented cells could be run separately. Analyzed volume was 100 ul. Unpigmented cells were stained with Hoechst stain at a final concentration of 1 µg mL-1. Abundances of each cell type were estimated by binning populations using FlowJo (v. 6.4.7) software.
Surface and reef depth seawater samples were also collected to quantify the concentrations of known metabolites and survey trends in untargeted metabolite feature composition using liquid chromatography mass

spectrometry. Detailed methods are included on the MetaboLights project page (Project MTBLS1820) and within the open access paper.

Data Processing Description

Abundances of each cell type were estimated by binning populations using FlowJo (v. 6.4.7) software.

BCO-DMO Curation Notes

Version 1:
* 908026_v2_biogeochemistry.csv was imported into the BCO-DMO data system with values "NaN" as missing data values. This file version was submitted to BCO-DMO 2023-10-26.
* The table was renamed 908026_v1_biogeochemistry in the BCO-DMO system since it will be the first published version of this dataset.
** Missing data values are displayed differently based on the file format you download. They are blank in csv files, "NaN" in MatLab files, etc.
* date format changed to ISO format

[table of contents | back to top]

Data Files

File
908026_v1_biogeochemsitry.csv (Comma Separated Values (.csv), 3.66 KB) MD5:d9d6f5abc00b30e5907da59f063e0b7c Primary data table for dataset 908026 version 1.

[table of contents | back to top]

Related Publications

Apprill, A., & Rappé, M. (2011). Response of the microbial community to coral spawning in lagoon and reef flat environments of Hawaii, USA. Aquatic Microbial Ecology, 62(3), 251–266. doi:10.3354/ame01471
Methods

FlowJo software version 6.4.7 (2005, November 16). Tree Star, Inc., Ashland, OR, USA. Retrieved from http://v9docs.flowjo.com/html/version.html#6.4.7
Software

Hansell, D. A., & Carlson, C. A. (2001). Biogeochemistry of total organic carbon and nitrogen in the Sargasso Sea: control by convective overturn. Deep Sea Research Part II: Topical Studies in Oceanography, 48(8-9), 1649–1667. doi:10.1016/s0967-0645(00)00153-3 https://doi.org/10.1016/S0967-0645(00)00153-3
Methods

Weber, L., Armenteros, M., Kido Soule, M., Longnecker, K., Kujawinski, E. B., & Apprill, A. (2020). Extracellular Reef Metabolites Across the Protected Jardines de la Reina, Cuba Reef System. Frontiers in Marine Science, 7. doi:10.3389/fmars.2020.582161
Results

[table of contents | back to top]

Related Datasets

IsRelatedTo

Apprill, A., Kujawinski, E., Gray, L. (2023) **Sampling and accession information for extracellular reef seawater metabolites collected from the Jardines de la Reina reef-system, Cuba in November of 2017.** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 1) Version Date 2023-10-20 doi:10.26008/1912/bco-dmo.843270.1 [view at BCO-DMO]
Relationship Description: Data from the same study (Metabolights study id MTBLS1820). In both the biogeochemistry and metabolite datasets, water samples were collected from surface and benthic depths from the same reefs. Column "reef" in both datasets indicates the reef site identifier and reef sample depth. See methods for details of how each water sample was collected.

IsSupplementTo

Weber, L., Apprill, A. (2020) MTBLS1820: Extracellular reef metabolites across the protected Jardines de la Reina, Cuba reef-system. MetaboLights Database. Released 2020-11-30. Available at https://www.ebi.ac.uk/metabolights/MTBLS1820/

[table of contents | back to top]

Parameters

Parameter	Description	Units
reef	sample name of reef (site identifier and sample depth; "surf" for surface or "benthic" for reef depth).	unitless
site	Site identifier	unitless
date	Date of water sample collection in ISO 8601 format	unitless
latitude	sample site latitude	decimal degrees
longitude	sample site longitude	decimal degrees
depth	depth of sampling	meters (m)
biome	general habitat description	unitless
sampling_depth	Descriptive term for sampling depth; "surf" for surface or "benthic" for reef depth.	unitless
grouping	general geographic grouping of reef sites	unitless
DOC	Dissolved organic carbon	micro molar (uM)
DN	Dissolved nitrogen	micro molar (uM)
TOC	Total organic carbon	micro molar (uM)

TN	Total nitrogen	micro molar (uM)
Pro	Prochlorococcus cell abundance	cells per mL
Syn	Synechococcus cell abundance	cells per mL
Pico	Picoeukaryote cell abundance	cells per mL
Hbact	Unpigmented cell abundance	cells per mL
Totalcells	Summation of all cell types	cells per mL
PO4	Phosphate	micro molar (uM)
SI	Silicate	micro molar (uM)
NO2	Nitrite	micro molar (uM)
NO3	Nitrate	micro molar (uM)
NH4	Ammonium	micro molar (uM)
DON	Dissolved organic nitrogen	micro molar (uM)
TON	Total organic nitrogen	micro molar (uM)
Temp	Seawater temperature	degrees Celsius
pH	pH	pH scale
Sal	salinity	parts per thousand (ppt)
DO	Dissolved oxygen	mg per L
TchI	Total chlorophyll a	micrograms per L
TchItoPhaeo	Ratio of total chlorophyll a to phaeophytin concentrations	unitless

[table of contents | back to top]

Instruments

Dataset-specific Instrument Name	Altra flow cytometer
Generic Instrument Name	Flow Cytometer
Dataset-specific Description	To obtain cell counts, flow cytometry was conducted using a collinear analyses method and a UV wavelength of 488 nm on an Altra flow cytometer at the University of Hawaii. Each sample was divided so that pigmented, fluorescent cells and unpigmented cells could be run separately.
Generic Instrument Description	Flow cytometers (FC or FCM) are automated instruments that quantitate properties of single cells, one cell at a time. They can measure cell size, cell granularity, the amounts of cell components such as total DNA, newly synthesized DNA, gene expression as the amount messenger RNA for a particular gene, amounts of specific surface receptors, amounts of intracellular proteins, or transient signalling events in living cells. Description from: http://www.bio.umass.edu/micro/immunology/facs542/facswhat.htm

Dataset-specific Instrument Name	Shimadzu TOC-VCSH total organic carbon analyzer (Hansell & Carlson, 2001)
Generic Instrument Name	Shimadzu Total Organic Carbon Analyzer TOC-VCPH
Dataset-specific Description	Non-purgeable total organic carbon (TOC, unfiltered), dissolved organic carbon (DOC, 0.2 µm filtered), total nitrogen (TN, unfiltered), and total dissolved nitrogen (TDN, 0.2 µm filtered) concentrations were analyzed using a Shimadzu TOC-VCSH total organic carbon analyzer (Hansell & Carlson, 2001) with a TNM-1 module.
Generic Instrument Description	The Shimadzu Total Organic Carbon Analyzer TOC-VCPH is a PC-controlled, total organic carbon analyzer (high-sensitivity model), designed to measure total carbon (TC), inorganic carbon (IC), total organic carbon (TOC), and non-purgeable organic carbon (NPOC); an optional accessory enables the measurement of particulate organic carbon (POC) and total nitrogen (TN) as well. The instrument uses the 680 degrees Celsius combustion catalytic oxidation method to analyze aqueous samples, and optionally solid and gas samples.

Dataset-specific Instrument Name	Lambda 18, Perkin Elmer, Waltham, MA, USA
Generic Instrument Name	Spectrophotometer
Dataset-specific Description	Acetone (90%) was used to extract Chlorophyll a and phaeophytin and the optical density (OD) values were measured on a calibrated spectrophotometer using standard optics (Lambda 18, Perkin Elmer, Waltham, MA, USA).
Generic Instrument Description	An instrument used to measure the relative absorption of electromagnetic radiation of different wavelengths in the near infra-red, visible and ultraviolet wavebands by samples.

Dataset-specific Instrument Name	YSI Exo Sonde (Xylem Inc., Yellow Springs, OH, USA)
Generic Instrument Name	YSI EXO multiparameter water quality sondes
Dataset-specific Description	At each reef, CTD casts were completed (YSI Exo Sonde, Xylem Inc., Yellow Springs, OH, USA) to measure the physicochemical properties of the water column.
Generic Instrument Description	Comprehensive multi-parameter, water-quality monitoring sondes designed for long-term monitoring, profiling and spot sampling. The EXO sondes are split into several categories: EXO1 Sonde, EXO2 Sonde, EXO3 Sonde. Each category has a slightly different design purpose with the EXO2 and EXO3 containing more sensor ports than the EXO1. Data are collected using up to four user-replaceable sensors and an integral pressure transducer. Users communicate with the sonde via a field cable to an EXO Handheld, via Bluetooth wireless connection to a PC, or a USB connection to a PC. Typical parameter specifications for relevant sensors include dissolved oxygen with ranges of 0-50 mg/l, with a resolution of +/- 0.1 mg/l, an accuracy of 1 percent of reading for values between 0-20 mg/l and an accuracy of +/- 5 percent of reading for values 20-50 mg/l. Temp ranges are from-5 to +50 degC, with an accuracy of +/- 0.001 degC. Conductivity has a range of 0-200 mS/cm, with an accuracy of +/-0.5 percent of reading + 0.001 mS/cm and a resolution of 0.0001 - 0.01 mS/cm.

[table of contents | back to top]

Project Information

Signature exometabolomes of Caribbean corals and influences on reef picoplankton (Coral Exometabolomes)

Coverage: U.S. Virgin Islands

NSF Award Abstract:
Coral reefs are some of the most diverse and productive ecosystems in the ocean. Globally, reefs have declined in stony (reef-building) coral abundance due to environmental variations, and in the Caribbean this decline has coincided with an increase in octocoral (soft coral) abundance. This phase shift occurring on Caribbean reefs may be impacting the interactions between the sea floor and water column and particularly between corals and picoplankton. Picoplankton are the microorganisms in the water column that utilize organic matter released from corals to support their growth. These coral-picoplankton interactions are relatively unstudied, but could have major implications for reef ecology and coral health. This project will take place in the U.S. territory of the Virgin Islands (USVI) and will produce the first detailed knowledge about the chemical diversity and composition of organic matter released from diverse stony coral and octocoral species. This project will advance our understanding of coral reef microbial ecology by allowing us to understand how different coral metabolites impact picoplankton growth and dynamics over time. The results from this project will be made publically accessible in a freely available online magazine, and USVI minority middle and high school students will be exposed to a lesson about chemical-biological interactions on coral reefs through established summer camps. This project will also contribute to the training of USVI minority undergraduates as well as a graduate student.

Coral exometabolomes, which are the sum of metabolic products of the coral together with its microbiome, are thought to structure picoplankton communities in a species-specific manner. However, a detailed understanding of coral exometabolomes, and their influences on reef picoplankton, has not yet been obtained. This project will utilize controlled aquaria-based experiments with stony corals and octocorals, foundational species of Caribbean reef ecosystems, to examine how the exometabolomes of diverse coral species differentially influence the reef picoplankton community. Specifically, this project will capitalize on recent developments in mass spectrometry-based metabolomics to define the signature exometabolomes of ecologically important and diverse stony corals and octocorals. Secondly, this project will determine how the

exometabolomes of these corals vary with factors linked to coral taxonomy as well as the coral-associated microbiome (Symbiodinium algae, bacteria and archaea). With this new understanding of coral exometabolomes, the project will then apply a stable isotope probe labeling approach to the coral exometabolome and will examine if and how (through changes in growth and activity) the seawater picoplankton community incorporates coral exometabolomes from different coral species over time. This project will advance our ability to evaluate the role that coral exometabolomes play in contributing to benthic-picoplankton interactions on changing Caribbean reefs.

RAPID/MRI: Acquisition of a Triple-Quad Mass Spectrometer for Quantitative Identification of Dispersants and Water-Soluble Oil in the Gulf of Mexico (RAPID Mass Spec for Dispersants)

Coverage: Gulf of Mexico

The PI's request MRI RAPID funding to acquire a triple-quad Mass Spectrometer for quantitative identification of dispersants and water-soluble oil in the Gulf of Mexico. Dispersants were applied to the leak at the bottom of the ocean. Preliminary results using the PI's Fourier-transform ion cyclotron resonance (FT) mass spectrometer show that is possible identify the active ingredient of this dispersant in samples collected during research cruises in the Gulf of Mexico. Components of the dispersant have even been found in samples taken from within the underwater oil plume deep below the ocean's surface (~1100 m). Now the PI's would like to quantify this compound in order to assess its environmental fate in this environment.

In order to quantify these marker compounds, a mass spectrometer designed for sensitive and accurate quantification of targeted compounds is required. The PI's have identified a triple-quadrupole mass spectrometer (triple-Q-MS) as the most appropriate instrument for their needs. With the help of the EPA, the PI's now have the appropriate method ready and have been running samples on a triple-Q-MS in a colleague's lab. The increased sensitivity and quantitative accuracy of the triple-Q-MS will allow them to quantify dispersant components and other target compounds at lower concentrations, thus providing important constraints on modeling and predictive efforts underway in other research groups.

Broader Impacts

This research has the potential to provided unprecedented data on the environmental fate of both petroleum and dispersant components as they interact with the extant biological, chemical, and physical processes of the Gulf of Mexico. Beyond the immediate needs of the Gulf oil spill the development of the methods described in the proposal will have broad applications not only in oil spill research but also in marine organic matter characterization and its interactions with biological, chemical and physical processes. The instrument will be available for Gulf oil spill related research in a timeframe consistent with the intent of the RAPID funding mechanism.

[table of contents | back to top]

Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1736288
NSF Division of Ocean Sciences (NSF OCE)	OCE-1058448

[table of contents | back to top]