Sampling and accession information for extracellular reef seawater metabolites collected from the Jardines de la Reina reef-system, Cuba in November of 2017

Website: https://www.bco-dmo.org/dataset/843270
Data Type: Other Field Results
Version: 1
Version Date: 2023-10-20

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
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Kujawinski, Elizabeth	Woods Hole Oceanographic Institution (WHOI)	Co-Principal Investigator
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Abstract
This dataset contains sampling and accession information for extracellular reef seawater metabolites collected from two different depths across 9 different shallow forereefs in the Jardines de la Reina reef-system, Cuba. Reef seawater samples, collected in duplicate per depth and location, were subjected to targeted and untargeted liquid chromatography mass spectrometry (LC-MS) methods in addition to a suite of biogeochemical measurements (see Related Datasets for access to the biochemistry data). Raw and .mzML data files from the LC-MS methods are located at MetaboLights database, using accession number MTBLS1820.(Accessible from https://www.ebi.ac.uk/metabolights/MTBLS1820/). These data were published in Weber et al. (2020).

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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 procedure summary:

Reef seawater microbial biogeochemistry and extracellular metabolite compositions 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).

Methods and data access for the biogeochemistry data are available from Related Dataset "Extracellular reef seawater biogeochemistry from the Jardines de la Reina reef-system" (see "Related Datasets" section).

Surface and reef depth seawater samples were also collected to quantify concentrations of known metabolites using a targeted metabolomics method and survey trends in untargeted metabolite feature composition using an untargeted method. Exometabolite extracts were subjected to reverse-phase liquid chromatography mass spectrometry after filtering and solid-phase- extraction.
Note: term "benthic" and "reef depth" are used interchangeably in columns "reef" and "Depth"

Targeted metabolomics analysis was completed using a UPLC (Accela Open Autosampler and Accela 1250 Pump, Thermo ScientificTM) coupled to a heated electrospray ionization source (H-ESI) and a triple stage quadrupole mass spectrometer (TSQ Vantage, Thermo Fisher ScientificTM), operated in selective reaction monitoring (SRM) mode. For chromatography, a Waters Acquity HSS T3 column (2.1 mm × 100 mm, 1.8 µm), equipped with a Vanguard pre-column, was used for chromatographic separation at 40 °C.

Untargeted metabolomics analysis was completed using an ultra-high performance liquid chromatography system (Vanquish UHPLC, Thermo ScientificTM) coupled with an Orbitrap Fusion Lumos Tribid mass spectrometer (Thermo ScientificTM) using the same chromatographic conditions as used for targeted metabolomics.

Detailed methods are included on the MetaboLights project page (Project MTBLS1820) and within the open access paper, Weber et al. (2020).

BCO-DMO Processing Description

BCO-DMO Data Manager Processing Notes:
* Sheet 1 of file "Cuba2017_metabdata_BCODMO_date_latlong.xlsx" was imported into the BCO-DMO data system with values "NaN" as missing data values. This file version was submitted to BCO-DMO 2023-09-06.
** Missing data values are displayed differently based on the file format you download. They are blank in csv files, "NaN" in MatLab files, etc.
* Column names adjusted to conform to BCO-DMO naming conventions designed to support broad re-use by a variety of research tools and scripting languages. [Only numbers, letters, and underscores. Can not start with a number]
* date format changed to ISO format
* Column "MetaboLights_Study_Number" was added with value "MTBLS1820" as discussed with submitter.
* Column "reef" and "site" added to correspond to related dataset, biogeochemistry data column "reef". See related dataset description. Reef values added from information in the sample identifier. Logic and the resulting reef column was reviewed by the submitter.

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Data Files

File
MTBLS1820 samples filename: 843270_v1_mtbls1820_samples.csv (Comma Separated Values (.csv), 24.85 KB) MD5:0ed217f36cf305fbc0ef1d288f4e26e8 Primary data table for dataset 843270 version 1. MTBLS1820 is the study identifier in the associated Metabolights repository.

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Related Publications

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

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Related Datasets

IsRelatedTo

Apprill, A., Kujawinski, E., Gray, L. (2023) **Reef seawater biogeochemistry data from samples collected in 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 2023-10-26 doi:10.26008/1912/bco-dmo.908026.1 [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/

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Parameters

Parameter	Description	Units
MetaboLights_Study_Number	MetaboLights study number	unitless
Sample_Name	Name of sample	unitless
reef	sample name of reef (site identifier and sample depth; "surf" for surface or "benthic" for reef depth).	unitless
site	Site identifier	unitless
Seawater_collection_date	Date of sample collection	unitless
Latitude	sampling location latitude	decimal degrees
Longitude	sampling location longitude	decimal degrees
Sample_type	sample type	unitless
Seawater_sampling_location	description of sampling location relative to the coral reef	unitless
Depth	categorical sampling depth (e.g. pooled QC, reef depth, surface)	unitless
Replicate	Indicates if a duplicate sample was collected for this location and depth	unitless
Profiling_mode	Type of method used - either targeted or untargeted	unitless
Ion_mode	Type of ionization used - either positive or negative	unitless
raw_file_name	full file name for the raw data file that can be downloaded from MetaboLights (extension .raw)	unitless
derived_file_name	full file name for the derived data file that can be downloaded from MetaboLights (extension .mzML)	unitless

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Instruments

Dataset-specific Instrument Name	Orbitrap Fusion Lumos (Thermo Fisher Scientific)
Generic Instrument Name	Mass Spectrometer
Dataset-specific Description	Mass spectrometry samples were analyzed on a Vanquish UHPLC system (Thermo Fisher Scientific) coupled via heated electrospray ionization (H-ESI) to an ultrahigh resolution tribrid mass spectrometer, the Orbitrap Fusion Lumos (Thermo Fisher Scientific).
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.

Dataset-specific Instrument Name	Thermo Scientific TSQ Vantage Triple Stage Quadrupole Mass Spectrometer
Generic Instrument Name	Mass Spectrometer
Dataset-specific Description	Extracts prepared for targeted metabolomics were analyzed using UPLC (Accela Open Autosampler and Accela 1250 Pump, Thermo Scientific) coupled to a heated electrospray ionization source (H-ESI) and a triple stage quadrupole mass spectrometer (TSQ Vantage, Thermo Fisher Scientific), operated in selective reaction monitoring (SRM) mode.
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.

Dataset-specific Instrument Name	Vanquish UHPLC system (Thermo Fisher Scientific)
Generic Instrument Name	Ultra high-performance liquid chromatography
Dataset-specific Description	Mass spectrometry samples were analyzed on a Vanquish UHPLC system (Thermo Fisher Scientific) coupled via heated electrospray ionization (H-ESI) to an ultrahigh resolution tribrid mass spectrometer, the Orbitrap Fusion Lumos (Thermo Fisher Scientific).
Generic Instrument Description	Ultra high-performance liquid chromatography: Column chromatography where the mobile phase is a liquid, the stationary phase consists of very small (< 2 microm) particles and the inlet pressure is relatively high.

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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.

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Funding

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

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