Mass-to-charge ratio +1 values in microbial cultures (Phaeodactylum tricornutum and cocultures) detected by proton transfer reaction time-of-flight mass spectrometer in 2021 and 2022

Website: https://www.bco-dmo.org/dataset/871602
Data Type: experimental
Version: 1
Version Date: 2022-03-18

Project
» Interactions between phytoplankton and bacterioplankton mediated by volatile organic compounds (Plankton Interactions and VOC)

Contributors	Affiliation	Role
Halsey, Kimberly	Oregon State University (OSU)	Principal Investigator
Giovannoni, Stephen	Oregon State University (OSU)	Co-Principal Investigator
York, Amber D.	Woods Hole Oceanographic Institution (WHOI BCO-DMO)	BCO-DMO Data Manager

Abstract
Mass-to-charge ratio (m/z) +1 values in microbial cultures (Phaeodactylum tricornutum and cocultures) were detected by proton transfer reaction time-of-flight mass spectrometer following methods in Moore et al. (2020). doi:10.1111/1462-2920.14861

Table of Contents

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

Coverage

Temporal Extent: 2021-01 - 2022-01

Dataset Description

See the "Related Datasets" section for more data from this study with Synechococcus WH8102.

PTR ToF-MS in the name of this dataset refers to proton-transfer reaction time-of-flight mass spectrometry (PTR-TOF/MS).

Methods & Sampling

Methodology:

Volatile organic compounds (VOCs) were sampled and measured using dynamic stripping chambers coupled to a proton transfer reaction time-of-flight mass spectrometer (Moore et al. 2020). VOC concentrations (ppbv) are exported directly from the PTR-MS Viewer 3.2.1.2 software (Ionicon Analytik GmbH, Innsbruck, Austria) into .txt files. Air concentrations for each m/z (+1) detected are reported already corrected for mass calibration, transmission efficiencies, and primary ion signals. Data include experiment, culture conditions, and flow conditions. 2-point calibration mode, 0.3 m/z search range, cycle 1000, and using an average of 10 spectra.

Sampling and analytical procedures:
Samples are measured directly from cultures or media blanks. Culture conditions are given as the growth phase (exponential or stationary phase). Cell densities are provided. The protocol is well described in Moore et al. (2020).

Media recipe:
Artificial seawater + 882 µM NO3 + 36.2 µM PO4 + 106 µM Si + 1x f/2 Trace metal mix + 1 x f/2 Vitamin mix

Data Processing Description

VOC concentrations (ppbv) are exported directly from the PTR-MS Viewer 3.4.4 software (Ionicon Analytik GmbH, Innsbruck, Austria) into .txt files. Air concentrations for each m/z (+1) detected are reported already corrected for mass calibration, transmission efficiencies, and primary ion signals.

BCO-DMO Curation Notes

BCO-DMO Data Manager Processing Notes:
* Data from source file "P.tricorn and cocultures data repositoryv3.xlsx", all sheets starting with name "Sample_*", were imported into the BCO-DMO data system and combined into one data table.
* Information from sheet "Sample Information" added to metadata text on this page, and a supplemental data table titled "Sample Information: Phaeodactylum tricornutum and cocultures" added to the Supplemental File section of this page.
* Values "NA" in the source file were classified as missing data identifiers.
* Parameters (column names) renamed to comply with BCO-DMO naming conventions. See https://www.bco-dmo.org/page/bco-dmo-data-processing-conventions
* Data table unpivoted. Format of the data table converted from wide form where there were data columns for each mz_value containing mz_signals. Converted to long format data table where there is a column "mz_value" and a column "mz_signal."
* Data table sorted by {Sample_Name}{Sample_Replicate}{Sample_Tech}{mz_value}{Time_seconds}
* Missing data values (Blank/Null) values in this dataset are displayed according to the format of data you access. For example, in csv files it will be blank values. In Matlab .mat files it will be NaN values. When viewing data online at BCO-DMO, the missing value will be shown as "nd" meaning "no data." See https://www.bco-dmo.org/page/bco-dmo-data-processing-conventions
* After discussion with the submitter, sample name "SatppiaARW1T_PT_coculture" changed to "StappiaARW1T_PT_coculture"
* taxa and taxon ids associated with each sample name reviewed by submitter and attached as a supplemental file.
* Time_seconds rounded to tenth decimal place.

[table of contents | back to top]

Data Files

File	
871602_v1_mz-p-trico-and-cocultures.csv	(Comma Separated Values (.csv), 34.77 MB) MD5:3194ce4d3ac6d63f33d718e7e8fcb325
Primary data file for dataset ID 871602, version 1	

[table of contents | back to top]

Supplemental Files

File
Sample Information: Phaeodactylum tricornutum and cocultures filename: sample_info_P_trico_adn_cocultures.csv (Comma Separated Values (.csv), 1.12 KB) MD5:32b7297984e4de8c9bbe5d19c4b6824c Additional sample metadata. Columns: Filename Sample Name Sample type Light (µEin/m2/s) Light: dark Temperature (Celcius) Media Flow (ml/min) Ion Mode Replicates Growth Phase Cell_density (Cells/ml)
Taxon list with identifiers filename: taxon_ids.csv (Comma Separated Values (.csv), 669 bytes) MD5:b756ac068ba04f5556972098eaac8576 Table with the sample name as it appears in the dataset, the associated taxon and identifiers. Columns: name_in_dataset, Sample name as it appears in the dataset taxon, taxon associated with the name in the dataset AphiaID, taxon identifier for the taxon. Aphia ID, see World Register of Marine Speices (WoRMS) for more information. LSID, Lifescience Identifier for the taxon

[table of contents | back to top]

Related Publications

IONICON (2022). PTR-MS Viewer: Data Visualization and Exploration. Accessed March 3rd, 2016. https://www.ionicon.com/accessories/details/ptr-ms-viewer
Software

Moore, E. R., Davie-Martin, C. L., Giovannoni, S. J., & Halsey, K. H. (2020). Pelagibacter metabolism of diatom-derived volatile organic compounds imposes an energetic tax on photosynthetic carbon fixation. Environmental Microbiology, 22(5), 1720–1733. Portico. https://doi.org/10.1111/1462-2920.14861
Results

[table of contents | back to top]

Related Datasets

IsRelatedTo

Halsey, K., Giovannoni, S. (2024) **Mass-to-charge ratio +1 values in microbial cultures (Synechococcus WH8102) detected by proton transfer reaction time-of-flight mass spectrometer in 2021 and 2022.** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 1) Version Date 2022-03-18 doi:10.26008/1912/bco-dmo.871678.1 [view at BCO-DMO]

[table of contents | back to top]

Parameters

Parameter	Description	Units
Sample_Name	Microbe in culture or coculture with Phaeodactylum tricornutum	unitless
Sample_Name_internal	Internal reference for culture	unitless
Sample_Replicate	Biological replicate	unitless
Sample_Tech	Technical replicate	unitless
Time_seconds	time of sampling period (seconds)	seconds (s)
mz_value	Mass-to-charge (m/z) +1 value identified by PTR-MS. This is the atomic mass plus 1 for a chemical compound detected by the mass spectrometer.	unitless
mz_signal	Mass-to-charge (m/z) signal	parts per billion by volume (ppbv)

[table of contents | back to top]

Instruments

Dataset-specific Instrument Name	TOF-1000
Generic Instrument Name	Mass Spectrometer
Dataset-specific Description	Proton transfer reaction time of flight mass spectrometer. Ionicon Analytik, Innsbruck, Austria. TOF-1000.
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.

[table of contents | back to top]

Project Information

Interactions between phytoplankton and bacterioplankton mediated by volatile organic compounds (Plankton Interactions and VOC)

NSF Award Abstract:
Communication amongst plants and animals often occurs through molecules that readily evaporate at normal temperatures, called volatile organic compounds (VOCs). Some VOCs that are produced in the ocean and then

enter the atmosphere as gases have been seen to play an important role in climate. Since marine microbes both produce and consume these compounds they affect the concentration of VOCs in the surface ocean. The investigators found that as much as 20% of the carbon resulting from photosynthesis leaked out of microscopic plants in the form of VOCs. These molecules were then used by bacteria as a source of carbon and energy. This suggests that VOCs may play a more important role in the flow of carbon in the marine environment than previously thought. This project examines how microscopic plants and bacteria produce and consume different VOCs. It supports professional development training workshops for Oregon high school teachers from rural areas in OSU's Science & Math Investigative Learning Experiences (SMILE) program. SMILE's mission is to close the achievement gap for underserved students by increasing their STEM-content knowledge, preparing them to succeed in higher education, and inspiring them to pursue STEM careers. This project also contributes to three workshops per year, training teachers and engaging students with hands-on learning activities on the topic of Carbon Cycling by Marine Microorganisms such as "Clouds in a Bottle". One graduate student, one post-doctoral scholar, and at least six undergraduate researchers are being trained by participating in research activities.

Field observations suggest that volatile organic compounds (VOCs) produced by phytoplankton are either rapidly consumed by bacterioplankton in the surface ocean or emitted into the atmosphere. VOCs are an understudied path for carbon transfer in microbial food webs throughout sunlit marine ecosystems because these compounds require specialized detection methods. Using a new system to study VOCs in suspensions of live plankton cells, 20% of photosynthetic carbon fixation was seen to be transferred as VOCs from a diatom to SAR11 bacterioplankton in co-cultures. Many of these transferred VOC compounds were not known to be growth substrates for bacterioplankton. Both the magnitude and complexity of the observed VOC transfer were surprising. This project extends these observations to a larger set of phytoplankton and bacterioplankton through controlled studies of cultures, co-cultures, and mesocosms. VOC are detected via proton transfer reaction time-of-flight mass spectrometry and isotopic labeling is used to measure the impact of VOC exchange on rates of photosynthesis and bacterial production. VOC production by phytoplankton is measured in response to nutrient-driven variation in growth rates, and over day-night cycles to discern the relationship of VOC production to photosynthetic metabolism and other cellular processes. These experiments enable a better understanding of field observations, in which bacterial consumption of VOCs can appear to significantly outpace production, while temporal variability in VOC production across daily to seasonal scales can cause VOCs to accumulate transiently to pM-nM concentrations in the surface ocean. This project contributes to close the significant gap in knowledge about the range and quantity of VOCs produced by phytoplankton, and about the roles played by these compounds in phytoplankton metabolism.

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.

[table of contents | back to top]

Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1948163

[table of contents | back to top]