Intracellular sulfonate metabolites measured in a variety of eukaryotic and prokaryotic phytoplankton and heterotrophic bacteria using liquid chromatography-mass spectrometry-based metabolomics

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Data Type: experimental
Version: 1
Version Date: 2020-06-10

Project
» OCE-PRF Track 1 (Broadening Participation): Cryptic Sulfonate Cycling between Marine Phytoplankton and Heterotrophic Bacterioplankton (Sulfonate Cycling)

Contributors	Affiliation	Role
Durham, Bryndan P.	University of Washington (UW)	Principal Investigator
Rauch, Shannon	Woods Hole Oceanographic Institution (WHOI BCO-DMO)	BCO-DMO Data Manager

Abstract
Intracellular sulfonate metabolites were measured in a variety of eukaryotic and prokaryotic phytoplankton and heterotrophic bacteria using liquid chromatography-mass spectrometry-based metabolomics. These data have been published in Durham et al. (2019). Raw data are available at Metabolomics Workbench under Project ID PR000797.

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Dataset Description

Intracellular sulfonate metabolites were measured in a variety of eukaryotic and prokaryotic phytoplankton and heterotrophic bacteria using liquid chromatography-mass spectrometry-based metabolomics. These data have been published in Durham et al. (2019). Raw data are available at Metabolomics Workbench under Project ID PR000797.

Methods & Sampling

Pure cultures of bacteria and phytoplankton were grown in artificial seawater medium, and cells were collected during mid-to-late exponential phase by gentle filtration onto 0.2 micron Durapore filters. All filters were flash frozen in liquid nitrogen and stored at -80 degrees Celsius until further processing. Frozen filters of cells and media blanks were extracted and analyzed using a targeted liquid chromatography-mass spectrometry-based metabolomics method according to the protocols in Boysen and Heal et al., 2018. Briefly, metabolites were extracted using a modified Bligh–Dyer extraction using 1:1 methanol/water (aqueous phase) and dichloromethane (organic phase). Targeted metabolomics data were generated using a Waters Xevo TQ-S triple quadrupole with both reverse-phase and hydrophilic interaction liquid chromatography (HILIC). Taurine, isethionate, sulfolactate, and cysteate were quantified using isotopically-labeled internal standards that were

added prior to extraction. DHPS was quantified by generating standard addition curves.

Instruments: Targeted metabolomics data were generated using a Waters Xevo TQ-S triple quadrupole (TQS) with electrospray ionization (ESI) in selected reaction monitoring mode (SRM) with polarity switching. SRM conditions for each compound (collision energy, cone voltage, precursor, and product ions) were optimized by infusion of each metabolite standard. For most metabolites, two SRM transitions were selected based on maximum peak areas. All chromatographic separations were carried out on a Waters Acquity I-Class UPLC (Waters Corporation, Milford, MA).

Data Processing Description

Data processing: Peak integration was performed using Skyline for small molecules. After integration, data were passed through an in-house quality control (QC) filter to ensure proper metabolite identification as described in Boysen et al. (2018).

BCO-DMO Processing:
- modified parameter names

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Data Files

File
sulfonates.csv (Comma Separated Values (.csv), 6.56 KB) MD5:8621872eb4c9e3d28a42199450f32112 Primary data file for dataset ID 814713

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Related Publications

Boysen, A. K., Heal, K. R., Carlson, L. T., & Ingalls, A. E. (2018). Best-Matched Internal Standard Normalization in Liquid Chromatography–Mass Spectrometry Metabolomics Applied to Environmental Samples. Analytical Chemistry, 90(2), 1363–1369. doi:10.1021/acs.analchem.7b04400
Methods

Durham, B. P., Boysen, A. K., Carlson, L. T., Groussman, R. D., Heal, K. R., Cain, K. R., … Armbrust, E. V. (2019). Sulfonate-based networks between eukaryotic phytoplankton and heterotrophic bacteria in the surface ocean. Nature Microbiology, 4(10), 1706–1715. doi:10.1038/s41564-019-0507-5
Results

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Related Datasets

IsDerivedFrom

Metabolomics Workbench. (2019). PR000797. Metabolomics Workbench. https://doi.org/10.21228/M8NT2T

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Parameters

Parameter	Description	Units
Organism	name and strain number	unitless
replicate	biological replicate	unitless
cells_filtered	number of cells extracted	unitless
DHPS	sulfonate	amol per cell
cysteic_acid	sulfonate	amol per cell
sulfolactate	sulfonate	amol per cell
isethionic_acid	sulfonate	amol per cell
taurine	sulfonate	amol per cell

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Instruments

Dataset-specific Instrument Name	Waters Xevo TQ-S triple quadrupole
Generic Instrument Name	Mass Spectrometer
Dataset-specific Description	Targeted metabolomics data were generated using a Waters Xevo TQ-S triple quadrupole with both reverse-phase and hydrophilic interaction liquid chromatography (HILIC).
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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Project Information

OCE-PRF Track 1 (Broadening Participation): Cryptic Sulfonate Cycling between Marine Phytoplankton and Heterotrophic Bacterioplankton (Sulfonate Cycling)

Coverage: University of Washington

NSF Award Abstract:
Information in the form of chemicals and energy flows constantly through complex networks of marine microbes. In the surface ocean, sunlight and atmospheric carbon dioxide are captured by autotrophic unicellular phytoplankton and transformed into a vast pool of organic matter that microbes use as metabolic currencies and signaling molecules to form the basis for different trading alliances. Several little-known sulfonate compounds have recently been identified as key currencies underlying marine bacterial-phytoplankton mutualisms and appear to be widespread in coastal communities. In this project, the fellow will investigate the prevalence and role of sulfonates in marine microbial interactions and their resulting impact on the Earth's biogeochemistry. With sponsor Dr. E. Virginia Armbrust at the University of Washington, the fellow will advance professionally through interdisciplinary training in microbial ecology and marine biogeochemistry. Broadening participation activities include mentorship of an undergraduate and development of an outreach program for a local minority-serving high school where students will conduct classroom laboratory exercises using microbiological and bioinformatics concepts.

Sulfonates are produced and degraded by several important phytoplankton and heterotrophic bacterial taxa, respectively. Yet, these compounds represent a poorly understood component of the marine organic matter pool. To the extent that sulfonates account for an unquantified flux of carbon and sulfur that supports mutualisms between bacteria and phytoplankton, sulfonates represent cryptic missing links in both carbon and sulfur transformations in the ocean. In this study, the fellow will use laboratory-based approaches to examine physiological and ecological controls on sulfonate production in model phytoplankton species and field-based approaches to examine taxonomically driven dynamics of sulfonate pools in the coastal waters of Puget Sound and surrounding North Pacific. Specifically, the fellow will perform metabolic profiling of model sulfonate-producing phytoplankton taxa (Aim I) and measure spatiotemporal gradients and turnover rates of sulfonates in the ocean environment using targeted in situ metabolite surveys (II) and stable isotope incubations (III), respectively, together with transcriptomics-based identification of marine microbes that control the fate of sulfonate-derived carbon (IV). The planned experiments will provide the first intensive characterization of sulfonates in the environment in terms of their contribution to the marine organic matter pool, their taxonomically driven spatiotemporal dynamics, and their roles in ocean ecosystem interdependencies.

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1521564

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