Results from lab number 5 from an LCMS inter-lab study of marine dissolved organic matter and algal extracts from analyses in May of 2021 that used both San Diego, CA seawater and laboratory cultures

Website: https://www.bco-dmo.org/dataset/859694
Version: 1
Version Date: 2021-08-27

Project
» The Metabolic Response of Coastal Bacteria to Mortality-Derived Phytoplankton Dissolved Organic Matter (MortalityDOM)

Contributors	Affiliation	Role
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Abstract
Results from one participating lab in a liquid chromatography–mass spectrometry (LC-MS) inter-lab study of marine dissolved organic matter and algal extracts. These results are from lab number 5 (Kujawinski) from analyses that took place in May of 2021 that used both seawater from Ellen Browning Scripps Memorial Pier, San Diego, CA, and cultures. The dataset from lab number 5 contains three types of files from 68 analytical runs on an Orbitrap Fusion Lumos mass spectrometer. There are three files for each run: one is a 'raw' file that is the vendor-specific format produced by the instrument, the second is an mzML file with only the MS1 peak information generated by ProteoWizard's msConvert tool, and the third type of file is an mzML file with the MS1 and MS2 peak information generated by ProteoWizard's msConvert tool. These are unprocessed data files that are available at MassIVE (http://dx.doi.org/10.25345/C5D25T) in order to allow computational analysis with the Global Natural Product Social Molecular Networking (GNPS) set of networking tools.

Table of Contents

Coverage

Spatial Extent: **Lat**:32.8663 **Lon**:-117.2546
Temporal Extent: 2021-02 - 2021-05

Methods & Sampling

Samples were provided by Jeffrey Hawkes from Uppsala University as part of an inter-lab comparison study which is being run by Hawkes, Daniel Petras (University of Tbingen), and Carsten Simon (ETH Zurich). The seven samples being analyzed include a quality control sample, a blank, a marine sample, an algal lysate, and three samples that are a combination of the marine sample and the algal lysate (A45M : 450 ppm A and 4500 ppm M; A15M: 150 ppm A and 4500 ppm M; A5M: 50 ppm A and 4500 ppm M).

The samples range from 100% seawater to 100% culture. The seawater was collected from the Ellen Browning Scripps Memorial Pier on the 26th of February 2021 between 11:00 and 19:00 PDT. That pier is here: 32.8663° N, 117.2546° W

See Supplemental Files section for further sample preparation procedures and details relevant to all labs participating in the study.

Kujawinski lab (lab 5) parameters:

Massive ID: MSV000087588

Mass Spec Type: Orbitrap Fusion Lumos

LC Type: UHPLC

Column Name: Waters Acquity HSS T3

Column Dimesions:2.1 x 100 mm, 1.8 um, 0.4

Gradient Length [min]: 10

Total Method length [min]: 17

Gradient: "5% to 50% B (7 min), 50% to 99% B (10 min), 99% to 99% B (13min), 5% to 5% B (17Min)"

-->MS1 parameters

Mass Range: 150-1500

MS1 Resolution: 500000

Micro Scans: 1

Max fill time MS1:200

AGC MS1: default

DDA Duty Cycle Time: ~1 sec

-->MS/MS parameters

Mass Range: 150-1500

MS1 Resolution: 120000

MS2 Resolution: 30000

Micro Scans: 1

Max fill time MS1: 100

Max fill time MS2: 100

AGC MS1: default

AGC MS2: default

Stepped collision energy: 20,30,40

MS/MS Threshold Absolute: 2.50E+04

TopN DDA: 5

Dynamic Exclusion: 5

DDA Duty Cycle Time: ~1 sec
Instruments:

The samples were analyzed on a Orbitrap Fusion Lumos. The instrument parameters were as follows:

Stationary phase: Waters Acquity HSS T3 column with 2.1 mm x 100 mm.

Particle size: 1.8m

Mobile phase: LC-MS grade water (A), acetonitrile (B) with 0.1% formic acid (FA) each.

Gradient: Start at 5% B, increase to 50% B at 7 min, increase to 99% B at 10 min, 3 min washout phase at 99% B, 4 min equilibration phase at 5% B (method length = 17 min).

Flow rate: 0.4 mL/min with a 5 ul injection.

Data Processing Description

Vendor-specific data files were converted to mzML files using msConvert.

mzML file parameters:

Mass range: 150 to 1500 m/z

MS1 mass resolution: 500000

Max fill time: 200 microseconds

MS1 Automatic Gain Control (AGC) = default

Data Dependent Duty Cycle Time ~ 1 second

Files submitted to MassIVE at the Center for Computational Mass Spectrometry under accession MSV000087588 "DOM LCMS-Interlab Study 2021 Lab5, version 2" (See Related Datasets section for full citation).

[table of contents | back to top]

Supplemental Files

File
Sample preparation and analysis guide filename: Inter-Lab-Comparison_MS-Settings.pdf (Portable Document Format (.pdf), 83.70 KB) MD5:e958f064598fbb2c10c6389ee39c1bed DOM_Interlab-LCMS study 2021 - Sample preparation and analysis guide (documentation version on 2021-10-08).
Study sample prep, step-to-step pipetting scheme filename: DOM-Interlab-Study_sample-prep-step-to-step.pdf (Portable Document Format (.pdf), 32.57 KB) MD5:5658698499b21bb2664b849c6280c197 DOM Inter-Lab MS/MS study sample preparation, step-to-step pipetting scheme (documentation version on 2021-10-08).
Study sample preparation filename: DOM-Interlab-Study_sample_prep.pdf (Portable Document Format (.pdf), 73.40 KB) MD5:21e7d873db295986d7a125e5943db44c DOM Inter-Lab MS/MS study sample preparation. This document contains sample processing details (documentation version on 2021-10-08).

[table of contents | back to top]

Related Datasets

IsRelatedTo

Longnecker, K., Kujawinski, E. B., & Soule, M. K. (2021). *MassIVE MSV000087588 - DOM LCMS-Interlab Study 2021 Lab5, version 2* [Data set]. MassIVE. https://doi.org/10.25345/C5D25T

[table of contents | back to top]

Parameters

Parameters for this dataset have not yet been identified

[table of contents | back to top]

Instruments

Dataset-specific Instrument Name	Orbitrap Fusion Lumos
Generic Instrument Name	Mass Spectrometer
Dataset-specific Description	The samples were analyzed on a Orbitrap Fusion Lumos. The instrument parameters were as follows: Stationary phase: Waters Acquity HSS T3 column with 2.1 mm x 100 mm. Particle size: 1.8µm Mobile phase: LC-MS grade water (A), acetonitrile (B) with 0.1% formic acid (FA) each. Gradient: Start at 5% B, increase to 50% B at 7 min, increase to 99% B at 10 min, 3 min washout phase at 99% B, 4 min equilibration phase at 5% B (method length = 17 min). Flow rate: 0.4 mL/min with a 5 ul injection.
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

The Metabolic Response of Coastal Bacteria to Mortality-Derived Phytoplankton Dissolved Organic Matter (MortalityDOM)

Coverage: Laboratory

NSF Award Abstract:
Microbes interact with one another through the exchange of chemicals dissolved in their surrounding waters. Decades of biochemical research have identified a small suite of chemicals that are required by microbes for growth and well-being. This limited suite is now being expanded with novel analytical tools based on mass spectrometry. In this project, the focus will be on chemicals that are released during the death of microbes, with particular attention paid to burst cells after viral infections and to the remnants of cells after grazing by protozoa (single celled organisms). These chemicals are not intentionally released by their producers, but they can still affect the growth and well-being of nearby bacteria and in turn the bacteria's ability to convert these molecules to carbon dioxide. The proposed comparison of the types and reactivities of chemicals released during the death of a brown tide alga will help improve models of carbon cycling in the coastal ocean. Two graduate students will be supported directly by this project. The proponent plans to teach two classes, one a

mass spectrometry course, the other an environmental metabolomics course. It is anticipated that as part of the evolution of the metabolomics course, data-training for metabolomics would become part of the course.

Microbial consortia are exquisitely sensitive to chemical changes in their surroundings and the diversity of microbial communities evolves with the composition of available growth substrates and nutrients. Thus, interactions between microbes, through the milieu of dissolved organic matter (DOM), lie at the heart of the global carbon cycle and thus merit significant study and investigation. This project focuses on the molecules that are released during microbial mortality through viral lysis or protozoan grazing. Using novel mass spectrometry-based tools, this project links the composition of dissolved organic matter derived from microbial mortality with the ability of heterotrophic bacteria to remineralize these substrates. Metabolic parameters and carbon transformation rates will be determined as a function of DOM source to assess the impact of DOM type on microbial physiology and carbon turnover. Laboratory results from model organisms will be compared to field settings where the model organisms dominate planktonic communities. The project will generate a suite of molecules that can be used in future experiments as markers of microbial mortality and will provide quantitative comparisons between the reactivity of viral lysate and grazer-derived DOM. These results will support improved parameterizations of microbial networks and their impact on the global carbon cycle.

[table of contents | back to top]

Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1634016

[table of contents | back to top]