Fourier transform ion cyclotron resonance mass spectrometer (FT-ICRMS) data from seasonal collections, Doboy Sound, Sapelo Island, GA, July and October 2014

Website: https://www.bco-dmo.org/dataset/735751
Data Type: Other Field Results
Version: 1
Version Date: 2018-05-10

Project
» High Resolution Linkages Between DOC Turnover and Bacterioplankton in a Coastal Ocean (SIMCO)

Contributors	Affiliation	Role
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Abstract
Dissolved organic matter (DOM) from field and incubation collections of Doboy Sounds estuarine waters near Sapelo Island, GA in July and October 2014 was analyzed for chemical composition. Analysis of the dissolved organic matter pool retrieved by solid-phase extraction (PPL resin) was analyzed to determine chemical formulas (by Fourier transform ion cyclotron resonance mass spectrometry, FT-ICR MS).

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Coverage

Temporal Extent: 2014-07 - 2014-10

Dataset Description

Dissolved organic matter (DOM) from field and incubation collections of Doboy Sounds estuarine waters near Sapelo Island, GA in July and October 2014 was analyzed for chemical composition. Analysis of the dissolved organic matter pool retrieved by solid-phase extraction (PPL resin) was analyzed to determine chemical formulas (by Fourier transform ion cyclotron resonance mass spectrometry, FT-ICR MS).

Methods & Sampling

DOM was collected in Doboy Sound off the southeastern U.S. in July and October 2014. Six 20 L carboys were filled with water and wrapped in black plastic. Three were processed immediately, while the remaining three were returned to Doboy Sound for a 24 h dark incubation before processing by an identical protocol. This experimental scheme was carried out twice during each sampling event, once at high tide (HT) and once at low tide (LT). Immediately after collection, samples were filtered (using 0.7 µm Whatman GF/F filters precombusted at 450°C for 5 h and pre-washed 0.2 µm Pall Supor membrane filters), and aliquots were stored frozen for DOC analysis. Filtrates were acidified to pH 2, and DOM was isolated using solid phase extraction (SPE) cartridges (Agilent Bond Elut PPL) as in Dittmar et al. (2008).

The molecular composition of the DOM extracts (200 mg C L-1 in methanol) was analyzed using a 9.4T Fourier transform ion cyclotron resonance mass spectrometer (FT-ICR MS) with electrospray ionization (ESI; negative mode) at the National ICR Users' Facility at the National High Magnetic Field Laboratory (NHMFL, Florida State University, Tallahassee, FL).

Assignment of molecular formulae was performed by Kendrick mass defect analysis (Wu et al., 2004) with PetroOrg software (Corilo, 2015) considering a maximum mass error of 0.5 ppm and using the criteria described by Rossel et al. (Rossel et al., 2013).

Data Processing Description

BCO-DMO Processing:
- added conventional header with dataset name, PI name, version date
- column names reformatted to comply with BCO-DMO standards

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Data Files

File
FTICRMS_2014.csv(Comma Separated Values (.csv), 1.09 MB) MD5:8d0efb4f0fc7bfc055a6bf5701ab8d3e Primary data file for dataset ID 735751

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Related Publications

Corilo, Y. (2015) PetroOrg Software; Florida State University: Tallahassee, FL, 2014.
Methods

Dittmar, T., Koch, B., Hertkorn, N., & Kattner, G. (2008). A simple and efficient method for the solid-phase extraction of dissolved organic matter (SPE-DOM) from seawater. Limnology and Oceanography: Methods, 6(6), 230–235. doi:10.4319/lom.2008.6.230
Methods

Rossel, P. E., Vähätalo, A. V., Witt, M., & Dittmar, T. (2013). Molecular composition of dissolved organic matter from a wetland plant (Juncus effusus) after photochemical and microbial decomposition (1.25 yr): Common features with deep sea dissolved organic matter. Organic Geochemistry, 60, 62–71. doi:10.1016/j.orggeochem.2013.04.013
Methods

Wu, Z., Rodgers, R. P., & Marshall, A. G. (2004). Two- and Three-Dimensional van Krevelen Diagrams: A Graphical Analysis Complementary to the Kendrick Mass Plot for Sorting Elemental Compositions of Complex Organic Mixtures Based on Ultrahigh-Resolution Broadband Fourier Transform Ion Cyclotron Resonance Mass Measurements. Analytical Chemistry, 76(9), 2511–2516. doi:10.1021/ac0355449
Methods

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Parameters

Parameter	Description	Units

mass_to_charge	mass-to-charge ratio (m/z). This is equivalent to the mass of a molecule since charge is 1	Daltons (Da)
C	number of carbon atoms in molecule	atoms
H	number of hydrogen atoms in molecule	atoms
O	number of oxygen atoms in molecule	atoms
N	number of nitrogen atoms in molecule	atoms
S	number of sulfur atoms in molecule	atoms
Jul14_HT_T0_A	relative abundance of molecule in sample Jul14_HT_T0_A	unitless
Jul14_HT_T0_B	relative abundance of molecule in sample Jul14_HT_T0_B	unitless
Jul14_HT_T0_C	relative abundance of molecule in sample Jul14_HT_T0_C	unitless
Jul14_HT_T24_A	relative abundance of molecule in sample Jul14_HT_T24_A	unitless
Jul14_HT_T24_B	relative abundance of molecule in sample Jul14_HT_T24_B	unitless
Jul14_HT_T24_C	relative abundance of molecule in sample Jul14_HT_T24_C	unitless
Jul14_LT_T0_A	relative abundance of molecule in sample Jul14_LT_T0_A	unitless
Jul14_LT_T0_B	relative abundance of molecule in sample Jul14_LT_T0_B	unitless
Jul14_LT_T0_C	relative abundance of molecule in sample Jul14_LT_T0_C	unitless
Jul14_LT_T24_A	relative abundance of molecule in sample Jul14_LT_T24_A	unitless
Jul14_LT_T24_B	relative abundance of molecule in sample Jul14_LT_T24_B	unitless
Jul14_LT_T24_C	relative abundance of molecule in sample Jul14_LT_T24_C	unitless
Oct14_HT_T0_A	relative abundance of molecule in sample Oct14_HT_T0_A	unitless

Oct14_HT_T0_B	relative abundance of molecule in sample Oct14_HT_T0_B	unitless
Oct14_HT_T0_C	relative abundance of molecule in sample Oct14_HT_T0_C	unitless
Oct14_HT_T24_A	relative abundance of molecule in sample Oct14_HT_T24_A	unitless
Oct14_HT_T24_B	relative abundance of molecule in sample Oct14_HT_T24_B	unitless
Oct14_HT_T24_C	relative abundance of molecule in sample Oct14_HT_T24_C	unitless
Oct14_LT_T0_A	relative abundance of molecule in sample Oct14_LT_T0_A	unitless
Oct14_LT_T0_B	relative abundance of molecule in sample Oct14_LT_T0_B	unitless
Oct14_LT_T0_C	relative abundance of molecule in sample Oct14_LT_T0_C	unitless
Oct14_LT_T24_A	relative abundance of molecule in sample Oct14_LT_T24_A	unitless
Oct14_LT_T24_B	relative abundance of molecule in sample Oct14_LT_T24_B	unitless
Oct14_LT_T24_C	relative abundance of molecule in sample Oct14_LT_T24_C	unitless

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Instruments

Dataset-specific Instrument Name	FT-ICR MS
Generic Instrument Name	Fourier Transform Ion Cyclotron Resonance Mass Spectrometer
Dataset-specific Description	The molecular composition of the DOM extracts were analyzed
Generic Instrument Description	In Fourier Transform Ion Cyclotron Resonance Mass Spectrometry, the mass-to-charge ratio (m/z) of an ion is experimentally determined by measuring the frequency at which the ion processes in a magnetic field. These frequencies, which are typically in the 100 KHz to MHz regime, can be measured with modern electronics making it possible to determine the mass of an ion to within +/- 0.000005 amu or 5 ppm.

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Project Information

High Resolution Linkages Between DOC Turnover and Bacterioplankton in a Coastal Ocean (SIMCO)

Coverage: Southeastern U.S. coastal ocean, 31.4° N Lat, 81.3° W Lon

Description from NSF award abstract:
Long-standing questions regarding the fate of dissolved organic carbon (DOC) in coastal oceans require a better understanding of the network that links bacterioplankton metabolism with carbon transformation. These questions address uncertainties about the composition of the bioreactive DOC components transformed in ocean margins, and the role of bacterial taxonomic and genetic composition in determining the fate of DOC.

This project will infuse a new type of data into coastal carbon cycle research based on high-resolution chemical analysis coupled with bacterial gene expression measures. It will extend DOC process studies down to the single-compound level and bacterial activity studies down to the single-gene level, and integrate this information into existing bioinformatic resources for biogeochemical and modeling applications.

The specific goals of this project are:
1) To reconstruct major components of the network linking DOC composition, DOC turnover, and bacterial heterotrophy in the coastal ocean (the composition of the DOC pool, the major bioreactive components, the bacterioplankton taxa mediating transformations, and the bacterial genes and pathways responsible).

2) To test hypothesized network links for selected DOC compounds using a simplified system that queries individual DOC compounds against a complex natural microbial community.

3) To test hypothesized network links for marine bacteria using a simplified system that queries a single generalist heterotrophic bacteria against a complex natural DOC pool.

4) To verify predicted DOC-gene linkages that are most informative about heterotrophic activities of bacterioplankton.

This research addresses fundamental questions on bacterial mediation of organic carbon fate in the ocean and atmosphere. As such, these investigations linking the chemical changes in dissolved organic carbon with patterns of gene expression in coastal bacterioplankton communities will be of interest to scientists across several disciplines.

Note: The project acronym, SIMCO, means "Sapelo Island Microbial Carbon Observatory".

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1356010

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