

# Fourier transform ion cyclotron resonance mass spectrometer (FT-ICR MS) data from seasonal collections, Doboy Sound, Sapelo Island, GA, 2012 and 2013

**Website:** <https://www.bco-dmo.org/dataset/661899>

**Data Type:** Other Field Results

**Version:**

**Version Date:** 2016-10-26

## Project

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

Contributors	Affiliation	Role
<a href="#">Moran, Mary Ann</a>	University of Georgia (UGA)	Principal Investigator
<a href="#">Medeiros, Patricia M.</a>	University of Georgia (UGA)	Co-Principal Investigator
<a href="#">Copley, Nancy</a>	Woods Hole Oceanographic Institution (WHOI BCO-DMO)	BCO-DMO Data Manager

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## Dataset Description

Field collected DOC from estuarine waters near Sapelo Island, GA in 2012 and 2013 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 November 2012, May 2013 and September 2013. At least 3 replicates were collected for each sample. Immediately after collection, samples were filtered (using 0.7  $\mu$ m Whatman GF/F filters pre-combusted at 450°C for 5 h and pre-washed 0.2  $\mu$ m 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).

DOC concentrations from water samples and extracts (i.e., dried and resuspended in ultrapure water) were measured with a Shimadzu TOC-VCPH analyzer. SPE efficiency across all samples was  $75 \pm 7\%$  of the DOC.

Bulk  $\delta$ -13C ratios of extracted DOC (SPE-DOC) were measured with a Finnigan MAT 251 isotope ratio mass spectrometer after complete drying. Precision and accuracy was better than 1 ppt, and procedural blanks did not yield detectable amounts of carbon isotopes. The molecular composition of the DOM extracts (15 mg C L<sup>-1</sup> in 1:1 methanol/water) was analyzed using a 15T Fourier transform ion cyclotron resonance mass spectrometer (FT-ICR MS; Bruker Daltonics) with electrospray ionization (negative mode) as in Seidel et al. (2014).

## Data Processing Description

### References:

Dittmar, T., Boris Koch, Norbert Hertkorn, and Gerhard Kattner. 2008. A simple and efficient method for the solid-phase extraction of dissolved organic matter (SPE-DOM) from seawater. *Limnol. Oceanogr.*: Methods 6, 2008, 230-235

Medeiros, P. M., M. Seidel, T. Dittmar, W. B. Whitman, and M. A. Moran (2015), Drought-induced variability in dissolved organic matter composition in a marsh-dominated estuary, *Geophys. Res. Lett.*, 42, 6446–6453, doi:10.1002/2015GL064653.

Seidel, M., Melanie Beck, Thomas Riedel, Hannelore Waska, I G.N.A. Suryaputra, d, Bernhard Schnetger, Jutta Niggemann, Meinhard Simonc, Thorsten Dittmar. 2014. Biogeochemistry of dissolved organic matter in an anoxic intertidal creek bank. *Geochimica et Cosmochimica Acta* 140:418-434.

<http://dx.doi.org/10.1016/j.gca.2014.05.038>

### BCO-DMO Processing:

- added conventional header with dataset name, PI name, version date
- column names reformatted to comply with BCO-DMO standards
- replaced spaces with underscores

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## Data Files

File
<b>FTICRMS.csv</b> (Comma Separated Values (.csv), 370.60 KB) MD5:ac2623b6c6f089ae6bab446b989acc9f Primary data file for dataset ID 661899

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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
P	number of phosphorous atoms in molecule	atoms
NOV_2012_A	relative abundance of molecule in sample Nov_2012_A	unitless
NOV_2012_B	relative abundance of molecule in sample Nov_2012_B	unitless
NOV_2012_C	relative abundance of molecule in sample Nov_2012_C	unitless
MAY_2013_A	relative abundance of molecule in sample May_2013_A	unitless
MAY_2013_B	relative abundance of molecule in sample May_2013_B	unitless
MAY_2013_C	relative abundance of molecule in sample May_2013_C	unitless
SEP_2013_A	relative abundance of molecule in sample Sep_2013_A	unitless
SEP_2013_B	relative abundance of molecule in sample Sep_2013_B	unitless
SEP_2013_C	relative abundance of molecule in sample Sep_2013_C	unitless

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## Instruments

<b>Dataset-specific Instrument Name</b>	FT-ICR MS (Bruker Daltonics)
<b>Generic Instrument Name</b>	Fourier Transform Ion Cyclotron Resonance Mass Spectrometer
<b>Dataset-specific Description</b>	The molecular composition of the DOM extracts were analyzed
<b>Generic Instrument Description</b>	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.

<b>Dataset-specific Instrument Name</b>	Finnigan MAT 251 isotope ratio mass spectrometer
<b>Generic Instrument Name</b>	Isotope-ratio Mass Spectrometer
<b>Dataset-specific Description</b>	Bulk delta-13C ratios of extracted DOC (SPE-DOC) were measured
<b>Generic Instrument Description</b>	The Isotope-ratio Mass Spectrometer is a particular type of mass spectrometer used to measure the relative abundance of isotopes in a given sample (e.g. VG Prism II Isotope Ratio Mass-Spectrometer).

<b>Dataset-specific Instrument Name</b>	Shimadzu TOC-VCPH analyzer
<b>Generic Instrument Name</b>	Shimadzu TOC-V Analyzer
<b>Dataset-specific Description</b>	DOC concentrations measured
<b>Generic Instrument Description</b>	A Shimadzu TOC-V Analyzer measures DOC by high temperature combustion method.

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## Deployments

### Moran\_Sapelo\_2012-14

<b>Website</b>	<a href="https://www.bco-dmo.org/deployment/661864">https://www.bco-dmo.org/deployment/661864</a>
<b>Platform</b>	Univ_Georgia
<b>Start Date</b>	2012-09-01
<b>End Date</b>	2014-10-31
<b>Description</b>	Microbial 'omics studies

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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.

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

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## Funding

Funding Source	Award
<a href="#">NSF Division of Ocean Sciences (NSF OCE)</a>	<a href="#">OCE-1356010</a>

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