Fourier Transform-Ion Cyclotron Resonance Mass spectrometry (FT-ICR MS) peaks lists from the Tapajós River, Brazil from 2016-2023

Website: https://www.bco-dmo.org/dataset/986858
Data Type: Other Field Results
Version: 1
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Project
» RAPID: El Nino Event Impacts on Organic Matter Export and Composition in the Amazon River (ENSO impact on Amazon River DOC and DOM)

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Abstract
This dataset includes assigned mass spectral peak lists from river water sampled near-monthly from the Tapajós River, Brazil between 2016-2023. Data were collected on a 21 T Fourier Transform-Ion Cyclotron Mass Spectrometer in electrospray negative ionization from solid phase DOM extracts. Trends in peak presence/absence and relative abundance reveal changes to DOM sourcing based on hydroclimate and multiyear climate anomalies.

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Coverage

Location: Tapajós River, Brazil
Spatial Extent: **Lat**:-4.3375 **Lon**:-56.06953
Temporal Extent: 2016-01-28 - 2023-11-30

Methods & Sampling

Water samples were collected near-monthly from the Tapajós River upstream of Itaituba Brazil (-4.3375,-56.06953). Three water samples (1 L) were collected at 0.5 m depth from the river across the channel in equal spacing and combined into a 4 L acid-washed carboy to make a composite sample. The water was filtered through a 0.45 µm capsule filter with a peristaltic pump into acid-rinsed high-density polyethylene (HDPE) bottles. Filtered samples were kept cold during transport and immediately frozen upon transfer to the laboratory and kept in the dark until analysis.

Data Processing Description

Mass spectral peaks (>6σ root-mean-square (RMS) baseline noise) were exported to a peak list and processed using PetroOrg. Molecular formulae were assigned to ions constrained by C4-75H4-150O1-30N0-4S0-2 not exceeding 300 ppb error. The resulting peak list includes all confidently assigned molecular formulae across every analyzed sample. Individual molecular formulae peaks can be compared between samples and bulk stoichiometric parameters (e.g., mean H/C , O/C ratio) can be determined for each sample in this dataset.

BCO-DMO Processing Description

* Sheet 1 of submitted file "Tapajos_FT-CR MS peaks_combined.csv" was imported into the BCO-DMO data system for this dataset. Table will appear as Data File: 986858_v1_tapajos_mass-spec-peaks.csv (along with other download format options).

* Data table within Sheet 1 from file "Tapajos_sample dates.xlsx" was imported as supplemental file (table added to BCO-DMO page as "sample-metadata.csv"). Column "Sample Name" was adjusted to add zero-padding for samples with only one digit in order to match to the primary data table column "Sample."
* sample date and lat,lon were added to the primary data 986858_v1_tapajos_mass-spec-peaks.csv by joining on the sample identifier in both tables.

Changes made in all tables in this dataset:

* Column names adjusted to conform to BCO-DMO naming conventions designed to support broad re-use by a variety of research tools and scripting languages. [Only numbers, letters, and underscores. Can not start with a number]

* Date converted to ISO 8601 format

* Location field contained both latitude and longitude in degrees minutes and seconds (e.g. '"4°20'15.0"S 56°04'10.3"W"') which was converted to separate lat_dd lon_dd columns (also converted to decimal degrees)

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Related Publications

Kurek, M. R., Muniz, R., Moura, J. M. S., Peucker-Ehrenbrink, B., Holmes, R. M., McKenna, A. M., & Spencer, R. G. M. (2025). Long-Term and Seasonal Drivers of Organic Matter in the Clearwater Tapajós River and Implications for the Amazon River Basin. Global Biogeochemical Cycles, 39(6). Portico. https://doi.org/10.1029/2025gb008545 https://doi.org/10.1029/2025GB008545
Results

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Related Datasets

IsRelatedTo

Kurek, M. (2025). Long-term and seasonal drivers of organic matter in the clearwater Tapajós River and implications for the Amazon River basin. *OSF*. https://doi.org/10.17605/OSF.IO/USH6Y

Kurek, M., Muniz, R., Moura, J. M., Peucker-Ehrenbrink, B., Holmes, R., McKenna, A., Spencer, R. (2026) **Absorbance and Excitation Emission spectra (EEMs) measurements of the Tapajós River, Brazil from 2016-2023.** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 1) Version Date 2026-01-20 http://lod.bco-dmo.org/id/dataset/986855 [view at BCO-DMO]
Relationship Description: Related datasets from the same study published in Kurek et al. (2025, doi: 10.1029/2025GB008545).

Kurek, M., Muniz, R., Moura, J. M., Peucker-Ehrenbrink, B., Holmes, R., McKenna, A., Spencer, R. (2026) **Dissolved organic matter, water quality, water isotopes, and discharge measurements of the Tapajós River, Brazil from 2016-2023.** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 1) Version Date 2026-01-20 http://lod.bco-dmo.org/id/dataset/986798 [view at BCO-DMO]
Relationship Description: Related datasets from the same study published in Kurek et al. (2025, doi: 10.1029/2025GB008545).

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Parameters

Parameter	Description	Units
Sample	Sample name	unitless
Date_ISO	Sample date in ISO 8601 format	unitless
lat_dd	Sample latitude	decimal degrees
lon_dd	Sample longitude	decimal degrees
Exp_mass	Experimental mass	Daltons (Da)
Theor_mz	Theoretical mass	Daltons (Da)
Error	Error between experimental and theoretical mass	parts per million (ppm)
Filez_RA	Peak relative intensity	unitless
DBE	Double bond equivalents	unitless
HC	H atoms/C atoms (ratio)	unitless
OC	O atoms/C atoms (ratio)	unitless

Molecular_Formula	Assigned molecular formula with all atoms	unitless
C	C (carbon) atoms	count
Hion	H (hydrogen)-1 ions (H- ion)	count
N	N (nitrogen) atoms	count
O	O (oxygen) atoms	count
S	S (sulfur) atoms	count
C13	13C (stable carbon isotope) atoms	count
H	H (hydrogen) atoms	count
P	P (phosphorous) atoms	count
AImod	Modified aromaticity index	unitless
NC	N atoms/C atoms	unitless
SC	S atoms/C atoms	unitless
NOSC	Nominal oxidation state of C (carbon)	unitless
Formula	Simplified molecular formula without isotopes	unitless
Class	Heteroatom-containing formula classification	unitless

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Instruments

Dataset-specific Instrument Name	FT-ICR mass spectrometer equipped with a 21T superconducting solenoid magnet at the National High Magnetic Field Laboratory (Tallahassee, FL)
Generic Instrument Name	Fourier Transform Ion Cyclotron Resonance Mass Spectrometer
Dataset-specific Description	Solid phase extracted water samples (PPL columns) were analyzed on a custom-built hybrid linear ion trap ultra-high resolution FT-ICR mass spectrometer equipped with a 21T superconducting solenoid magnet at the National High Magnetic Field Laboratory (Tallahassee, FL). Negatively charged ions from DOM were produced via electrospray ionization (ESI) at a flow rate of 500 nL min-1 via a syringe pump. Typical conditions for ion formation included: emitter voltage, -2.8–3.2 kV; S-lens RF level, 40%; and heated metal capillary temperature, 350 degrees C.
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

RAPID: El Nino Event Impacts on Organic Matter Export and Composition in the Amazon River (ENSO impact on Amazon River DOC and DOM)

Coverage: Amazon River basin

NSF Award Abstract:
The Amazon River is one of the largest sources of freshwater and carbon to the ocean. Thus, understanding the factors that influence freshwater delivery from the Amazon River is important for understanding the carbon cycle of the Amazon River and the receiving Atlantic Ocean. El Niño–Southern Oscillation (ENSO) is a periodic event that causes changes in winds and sea surface temperature over the tropical eastern Pacific Ocean and affects climate in the tropics and subtropics. The National Weather Service predicts that El Niño conditions are likely to form across the Pacific during Summer 2023. These conditions are expected to last through February 2024. This event is expected to impact precipitation and air temperatures in the Amazon Basin and freshwater delivery from the Amazon River. This project aims to study the amount and chemical composition of dissolved organic carbon delivered from the Amazon River to the Atlantic Ocean during the 2023-2024 El Niño event. Scientists involved in this project plan to collect samples from late Summer 2023 through late Summer 2024. The study will identify conditions before, during and after this event. This unique set of samples will enable the team of scientists to study how ENSO influences the delivery of organic carbon to the coastal ocean.
This project provides support for an early career researcher and promotes international cooperation and inclusivity between researchers from the United States of America and researchers in Brazil who are directly impacted by the changing Amazon River.

This project examines how El Niño Southern Oscillation (ENSO) anomalies impact the export of dissolved organic carbon (DOC) and composition of dissolved organic matter (DOM) from the Amazon River to the Atlantic Ocean. Based on recent studies, it has been hypothesized that the upcoming 2023 El Niño event will reduce the annual DOC flux and proportion of exported terrestrial DOM from the Amazon River compared to non-ENSO and La Niña years. This hypothesis will be examined by linking established state-of-the-art optical and molecular-level characterization techniques (e.g., Fourier-transform ion cyclotron resonance mass spectrometry; FT-ICR MS) with DOC flux calculations over the course of an El Niño year. Analyzing both bulk DOC fluxes and the molecular-level composition will reveal how the quantity and quality of DOM export will change monthly in response to reduced precipitation and higher temperature across the Amazon Basin and headwaters. DOC fluxes as well as detailed characterizations (FT-ICR MS, optical, fluorescence analysis) of

DOM sampled from the furthest downstream Amazon River gauging station at Óbidos (Brazil) will be directly compared to results obtained from the 2011-2012 La Niña year and the following 2012-2013 hydrologically normal year to determine how global climate anomalies impact the DOC export to marine systems and to create a framework for future predictions. Data obtained from this proposed study will lay the foundations for larger studies investigating how ENSO cycles impact discharge and carbon export from other major tropical-subtropical rivers and ultimately, how ENSO cycles impact global land-ocean carbon export.

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.

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-2333961

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