Biochemical data on dissolved organic matter composition from Galveston Bay collected on five one-day trips aboard R/V Trident following Hurricane Harvey from September 4 to 28, 2017

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Data Type: Cruise Results
Version: 1
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Project
» Collaborative Research: Distribution and Cycling of Carboxyl-Rich Alicyclic Molecules (CRAM) in the Ocean (CRAM in the ocean)

Contributors	Affiliation	Role
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Abstract
This dataset contains biochemical data on dissolved organic matter composition collected on five consecutive one-day trips aboard R/V Trident along a transect from the Port of Houston to the Galveston Bay entrance following Hurricane Harvey from September 4 to September 28, 2017.

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Coverage

Location: Galveston Bay, Texas, USA
Spatial Extent: **N**:29.6725 **E**:-94.6886 **S**:29.33278 **W**:-94.9789
Temporal Extent: 2017-09-04 - 2017-09-28

Methods & Sampling

Surface water samples were collected on five consecutive one-day trips aboard R/V Trident along a transect from the Port of Houston to the Galveston Bay entrance following Hurricane Harvey from September 4 to September 28, 2017. Samples were filtered on board through 0.2-micrometer (µm) Whatman-Nucleopore Q-TEC filters (Filtration Solutions) for dissolved organic carbon (DOC), optical, and chemical analysis.

Concentrations of DOC were measured by high-temperature catalytic oxidation using a Shimadzu TOC-V total organic carbon analyzer. Deep seawater reference standards (Consensus Reference Program, University of Miami) were used to assure the accuracy of DOC measurements. Absorbance was measured in a 1-centimeter (cm) quartz cuvette from 200 to 800 nanometers (nm) using a dual-beam spectrophotometer (UV-1800, Shimadzu) with Milli-Q water as the reference blank. Specific UV absorbance (SUVA254) was determined by dividing the UV absorbance at 254 nm by the DOC concentration. The spectral slope (S275−295) was calculated using the linear regression of natural log-transformed absorption spectra (Helms et al., 2008).

Samples for dissolved lignin (900 milliliters (mL)) were acidified to pH 2.5 using 6 moles per liter (mol L-1) sulfuric acid and extracted through Agilent PPL cartridges (1 gram (g)) at 10 milliliters per minute (mL min-1). After extraction, cartridges were rinsed with 10 mL of deionized water acidified to pH 2.5 and dried for 30 seconds to remove residual water. The cartridges were eluted with 20 mL of methanol at 2 mL min-1, and the eluate was stored in glass vials at -20 degrees Celsius until analysis. Concentrations of lignin phenols were determined using ultra-high performance liquid chromatography-electrospray ionization-tandem mass spectrometry after CuSO4 oxidation, following the methods described in Yan and Kaiser (2018a,b). Aliquots of methanol extracts (~30 microgram (µg) sample OC content) were dried in reaction vials and re-suspended in 200 microliters (µL) of 1.1 mol L-1 argon-sparged NaOH, followed by addition of 10 µL of 10 millimoles per liter (mmol L-1) CuSO4 and 10 µL of 0.2 mol L-1 ascorbic acid. Reaction vials were vigorously mixed and placed into 60-mL pressure-tight Teflon vessels filled with 5 mL of 1 mol L-1 NaOH. The oxidation was conducted at 150 degrees Celsius for 120 minutes. Sample solutions were spiked with 13C-labeled surrogate standards and purified with Waters HLB cartridges (30 milligram (mg), 1 mL). Separation and detection of lignin phenols was performed on an Agilent Infinity 1260 series UHPLC system coupled to an Agilent 6420 QqQ detector operating in alternating positive and negative modes with dynamic multiple reaction monitoring. Eleven lignin phenols were determined in all samples, including vanillyl phenols (V; vanillin, acetovanillone, and vanillic acid), syringyl phenols (S; syringaldehyde, acetosyringone, and syringic acid), p-hydroxyl phenols (P; p-hydroxybenzaldehyde, p-hydroxyacetophenone, and p-hydroxybenzoic acid), and cinnamyl phenols (C; p-coumaric acid and ferulic acid).

Total hydrolyzable enantiomeric dissolved amino acids (free and combined), including L-and D- forms of aspartic acid, glutamic acid, serine, histidine, threonine, glycine, arginine, alanine, tyrosine, valine, isoleucine, phenylalanine, leucine, and lysine were analyzed using high-performance liquid chromatography and fluorescence detection. After microwave-assisted vapor phase hydrolysis (Kaiser and Benner, 2005), amino acid monomers were derivatized with a mixture of N-isobutyryl- L-cysteine and o-phthaldialdehyde and separated on an Agilent Poroshell 120 EC-C18 column (4.6 millimeters (mm) × 100 mm, 2.7 µm). A binary solvent system was employed: mobile phase A was 48 mmol L-1 KH2PO4 with pH adjusted to 6.25, and mobile phase B was methanol/acetonitrile (13/1, v/v). The linear gradient program was: 0% B at 0 minutes, 39% B at 13.3 minutes, 54% B at 19.2 minutes, 60% B at 21.3 minutes, 80% B at 22 minutes, and hold at 80% B for 1 minute. The flow rate was 1.5 mL min-1 and column temperature was maintained at 35 degrees Celsius. Excitation and emission wavelength of the detector was set to 330 nm and 450 nm, respectively. Racemization of amino acid enantiomers occurring during acidic hydrolysis was corrected using the average rates determined on free and protein amino acids (Kaiser and Benner, 2005). Total D-amino acids (D-AA) was defined as the sum of the four D-enantiomers of aspartic acid (D-Asx), glutamic acid (D-Glx), serine (D-Ser), and alanine (D-Ala), which were ubiquitously present in all samples.

Data Processing Description

Instrument data were organized in Excel spreadsheets. Mass spectrometry data were processed with Matlab code provided in Fu et al. (2020). Final data were prepared with Anaconda Python distribution 2023.09-0, Python version 3.11.5.

BCO-DMO Processing Description

- Imported original file "Chemical_data_GB.csv" into the BCO-DMO system.
- Marked "NA" as a missing data value (missing data are empty/blank in the final CSV).
- Converted Date column to YYYY-MM-DD format.
- Renamed fields to comply with BCO-DMO naming conventions.
- Saved the final file as "982177_v1_coastal_dom_galveston_bay.csv".

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Related Publications

Helms, J. R., Stubbins, A., Ritchie, J. D., Minor, E. C., Kieber, D. J., & Mopper, K. (2008). Absorption spectral slopes and slope ratios as indicators of molecular weight, source, and photobleaching of chromophoric dissolved organic matter. Limnology and Oceanography, 53(3), 955–969. doi:10.4319/lo.2008.53.3.0955

Methods

Kaiser, K., & Benner, R. (2005). Hydrolysis-induced racemization of amino acids. Limnology and Oceanography: Methods, 3(8), 318–325. doi:10.4319/lom.2005.3.318
Methods

Yan, G., & Kaiser, K. (2018). A rapid and sensitive method for the analysis of lignin phenols in environmental samples using ultra-high performance liquid chromatography-electrospray ionization-tandem mass spectrometry with multiple reaction monitoring. Analytica Chimica Acta, 1023, 74–80. doi:10.1016/j.aca.2018.03.054
Methods

Yan, G., & Kaiser, K. (2018). Ultralow Sample Volume Cupric Sulfate Oxidation Method for the Analysis of Dissolved Lignin. Analytical Chemistry, 90(15), 9289–9295. doi:10.1021/acs.analchem.8b01867
Methods

Yan, G., Labonté, J. M., Quigg, A., & Kaiser, K. (2020). Hurricanes Accelerate Dissolved Organic Carbon Cycling in Coastal Ecosystems. Frontiers in Marine Science, 7. https://doi.org/10.3389/fmars.2020.00248
Results

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Parameters

Parameter	Description	Units
Date	Date sample was collected	unitless
Station	Site identification	unitless
Lat	Latitude	degrees
Long	Longitude	degrees
Salinity	Salinity	psu
DOC	Dissolved organic carbon	micromoles per liter (umol L-1)
a254	absorption coefficient at 254 nm	per meter (m-1)
SUVA	CDOM absorbance parameter	L mgC-1 m-1
S275_295	Spectral slope range 275-295 nm	unitless
S350_400	Spectral slope range 350-450 nm	unitless
SR	Spectral slope ratio 275-295/350-400	unitless
HIX	Humification Index (HIX); DOM composition metric	unitless

BIX	BIX; DOM composition metric	unitless
FI	Fluorescence Index (FI); DOM composition metric	unitless
C1	Fluorescence intensity of component 1	Raman units
C2	Fluorescence intensity of component 2	Raman units
C3	Fluorescence intensity of component 3	Raman units
C4	Fluorescence intensity of component 4	Raman units
PAL	p-hydroxy-benzaldehyde	nanomoles per liter (nmol L-1)
PON	p-hydroxy-acetophenone	nanomoles per liter (nmol L-1)
PAD	p-hydroxy-benzoic acid	nanomoles per liter (nmol L-1)
VAL	vanillin	nanomoles per liter (nmol L-1)
VON	acetovanillone	nanomoles per liter (nmol L-1)
VAD	vanillin acid	nanomoles per liter (nmol L-1)
SAL	syringealdehyde	nanomoles per liter (nmol L-1)
SON	acetosyringone	nanomoles per liter (nmol L-1)
SAD	syringic acid	nanomoles per liter (nmol L-1)
CAD	coumaric acid	nanomoles per liter (nmol L-1)
FAD	ferulic acid	nanomoles per liter (nmol L-1)
TDLP9	sum of 9 total dissolved lignin phenols	nanomoles per liter (nmol L-1)
P_V	[not provided]	[not provided]

S_V	[not provided]	[not provided]
C_V	[not provided]	[not provided]
Ad_AlV	[not provided]	[not provided]
Ad_AlS	[not provided]	[not provided]
His	histidine	nanomoles per liter (nmol L-1)
Thr	threonine	nanomoles per liter (nmol L-1)
Gly	glycine	nanomoles per liter (nmol L-1)
Arg	arginine	nanomoles per liter (nmol L-1)
Tyr	tyrosine	nanomoles per liter (nmol L-1)
Val	valine	nanomoles per liter (nmol L-1)
Ileu	isoleucine	nanomoles per liter (nmol L-1)
Phe	phenylalanine	nanomoles per liter (nmol L-1)
Leu	leucine	nanomoles per liter (nmol L-1)
Lys	lysine	nanomoles per liter (nmol L-1)
Ala	alanine	nanomoles per liter (nmol L-1)
Ser	serine	nanomoles per liter (nmol L-1)
Glx	glutamic acid and glutamine	nanomoles per liter (nmol L-1)
Asx	aspartic acid and asparagine	nanomoles per liter (nmol L-1)
DAA	sum of dissolved D-amino acids	nanomoles per liter (nmol L-1)

THAA	total hydrolyzable amino acids	nanomoles per liter (nmol L-1)

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Instruments

Dataset-specific Instrument Name	Agilent 6420 QqQ detector
Generic Instrument Name	Quadrupole Mass Spectrometer
Generic Instrument Description	A piece of apparatus that consists of an ion source, a mass-to-charge analyser, a detector and a vacuum system and is used to measure mass spectra. The detector is a quadrupole mass-to-charge analyser, which holds the ions in a stable orbit by an electric field generated by four parallel electrodes.

Dataset-specific Instrument Name	Shimadzu TOC-V total organic carbon analyzer
Generic Instrument Name	Shimadzu TOC-V Analyzer
Generic Instrument Description	A Shimadzu TOC-V Analyzer measures DOC by high temperature combustion method.

Dataset-specific Instrument Name	Agilent Infinity 1260 series UHPLC system
Generic Instrument Name	Ultra high-performance liquid chromatography
Generic Instrument Description	Ultra high-performance liquid chromatography: Column chromatography where the mobile phase is a liquid, the stationary phase consists of very small (< 2 microm) particles and the inlet pressure is relatively high.

Dataset-specific Instrument Name	dual-beam spectrophotometer (UV-1800, Shimadzu)
Generic Instrument Name	UV Spectrophotometer-Shimadzu
Generic Instrument Description	The Shimadzu UV Spectrophotometer is manufactured by Shimadzu Scientific Instruments (ssi.shimadzu.com). Shimadzu manufacturers several models of spectrophotometer; refer to dataset for make/model information.

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Project Information

Collaborative Research: Distribution and Cycling of Carboxyl-Rich Alicyclic Molecules (CRAM) in the Ocean (CRAM in the ocean)

NSF Award Abstract:
Collaborative Research: Distribution and Cycling of Carboxyl-Rich Alicyclic Molecules (CRAM) in the Ocean

Dissolved organic matter is the largest pool of organic carbon in the ocean. Thus, it plays an important role in carbon storage and climate change. The components of dissolved organic matter are the remains of biological products. As a result, the chemical make-up of dissolved organic matter (DOM) can provide important clues about the processes affecting this carbon pool. By learning more about the chemical structures and reactions that produce DOM, connections can be made to biological and biochemical processes and their importance. This project will study the distribution, production, and removal of one important class of molecules called carboxyl-rich alicyclic molecules (CRAM). These molecules are abundant in marine DOM and play an important role in the ocean carbon cycle. They also affect the supply of the micronutrient iron, and thus have an important influence on primary production and ocean food webs. The research includes field and laboratory experiments and takes advantage of ocean locations with long-term data. Together, the lead scientists will provide training and resources for the graduate students, undergraduate research opportunities for underrepresented groups in STEM, and direct outreach to the public through a website, articles in local newspapers, and talks at public venues.

CRAM make-up 8 to 25% of marine dissolved organic carbon (DOC) and represent a carbon reservoir of >65 Pg C that is equivalent to at least 8% of the atmospheric CO2 pool. CRAM play a central role in the functioning of the microbial carbon pump, a conceptual framework for producing refractory carbon by microbial processes in the ocean. Further, CRAM act as an important ligand of Fe(III) in the ocean, thereby playing an important role in regulating marine primary production. The main project objectives are: (1) measure the variable distribution of CRAM in the ocean, and (2) determine the dominant mechanisms of CRAM production and removal. The project will leverage an extensive set of already collected samples across the world’s oceans and new field work within the framework of the Bermuda Atlantic and Hawaii Ocean Time Series. Field measurements will be combined with experimental approaches to specifically address microbial and photochemical reactions leading to CRAM production and removal. This research will fill important gaps in resolving the key questions about organic carbon cycling in the ocean and explore the role of DOM in mediating the cycles of iron and other trace elements.

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-2148831

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