Dissolved organic carbon, and chromophoric and fluorescent DOM measurements of sea surface microlayer and subsurface samples from the R/V Hugh R. Sharp cruises HRS2213, HRS2215 and HRS2407 in the Northwestern Atlantic Ocean in 2022 and 2024

Website: https://www.bco-dmo.org/dataset/986840
Data Type: Cruise Results
Version: 1
Version Date: 2025-12-10

Project
» Collaborative Research: Impacts of surface ocean surfactant sources and transformations on their chemical composition and air-sea relevant properties (SOAPI)

Contributors	Affiliation	Role
Wozniak, Andrew S.	University of Delaware	Principal Investigator
Frossard, Amanda	University of Georgia (UGA)	Co-Principal Investigator
Agblemanyo, Felix Edufia	University of Delaware	Student
Ammer, Daniel	University of Georgia (UGA)	Student
Birt, Amber E.	University of Georgia (UGA)	Student
Rauch, Shannon	Woods Hole Oceanographic Institution (WHOI BCO-DMO)	BCO-DMO Data Manager

Abstract
Data includes dissolved organic carbon, as well as chromophoric and fluorescent dissolved organic matter (DOM) concentrations, of sea surface microlayer (SML) and subsurface samples collected across four hydrographic regions in the western North Atlantic. Sample information, including date and time, location (longitude and latitude), and oceanographic measurements such as salinity, temperature, wind speed, and humidity at the time of collection, is provided. SML samples were collected with a modified glass plate sampler, the Rosette-Based Glass Plate (RGP) Sampler, while subsurface samples were collected from a depth of 0.5 m using a pump. These data were generated as part of the Surfactants at the Ocean-Atmosphere Physical Interface (SOAPI) project to investigate the the composition, structure, and interfacial properties of surfactant organics at the sea surface. Data were collected by Dr. Andrew Wozniak (University of Delaware).

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Coverage

Location: Western North Atlantic
Spatial Extent: **N**:38.76335 **E**:-73.55657318 **S**:35.98858259 **W**:-75.435128
Temporal Extent: 2022-08-24 - 2024-08-19

Methods & Sampling

Sea surface microlayer (SML) samples were collected using the rosette-based glass plate sampler aboard the R/V Hugh R. Sharp. Subsurface seawater (SSW) was collected from the starboard side of the ship using a modified pump profiler system (Hudson et al. 2019) from ~0.5 meters (m) depth, immediately after each SML sampling. The samples were filtered using 0.7 micrometer (µm) pre-combusted glass fiber filters. An aliquot of filtered were frozen at -20 degrees Celsius (C) for DOC measurements, while another portion was stored in the fridge at 4 degrees C for colored dissolved organic matter (CDOM) and fluorescent dissolved organic matter (FDOM) analysis.

To measure dissolved organic carbon (DOC) concentrations, ~20 milliliters (mL) filtered water samples were acidified to a pH of ~2 using 4 drops of 2 molar (M) HCl. DOC was then quantified using the non-purgeable organic carbon method on a high temperature combustion instrument (Shimadzu TOC-V) that has a low blank (<5 micromolar (µM) C) and high precision (~1% RSD; (Qian and Mopper 1996)), following published studies (e.g., (Wozniak et al. 2012)). Sample responses were calibrated and validated against consensus surface seawater reference material from the Hansell laboratory at the University of Miami. DOC enrichment factors were calculated as a ratio of DOC concentration in the SML to DOC concentration in the paired SSW sample.

To characterize the optical properties of the SML and SSW DOM, both absorbance and excitation emission matrix (EEMs) fluorescence spectra were collected using a Horiba Aqualog spectrofluorometer. Absorbance spectra were acquired from 230 to 700 nanometers (nm) at 2 nm intervals. DOM aromaticity was estimated using SUVA254, which was calculated by dividing the absorption coefficient at 254 nm (a254) by DOC concentration (milligrams carbon per liter) (mg C L^{-1}). EEMs were obtained by scanning excitation wavelengths at 2 nm intervals between 230 and 700 nm, with emission spectra recorded at 4.65 nm intervals from 254 to 822 nm. The humification and biological indices (HIX and BIX) were calculated from the EEMs data using the *staRdom* and *eemR* R packages following standard procedures (Ohno 2002; Ouyang et al. 2024).

Additional measurements of the physical properties of seawater and meteorological conditions were made with the ship's instrumentation. Sea surface temperature and salinity were measured and recorded continuously with the shipboard instrumentation (SBE 45, Sea-Bird, at 3.7 m depth). Chlorophyll a concentrations were continuously measured with the shipboard fluorometer (AU10, Turner). Discrete water samples were also collected and used for chlorophyll a concentration measurements in the lab, using the spectrophotometric method described by Aminot and Rey (2000), to calibrate the shipboard fluorometer measurements. Wind velocity and air temperature were measured and recorded continuously with the ship's meteorological station (RM Young 26700).

BCO-DMO Processing Description

- Imported original file "SOAPI_1-3_DOC_CDOM.xlsx" into the BCO-DMO system.
- Renamed fields to comply with BCO-DMO naming conventions.
- For all columns except Latitude and Longitude, if more than 3 decimal places in numerical values, values were rounded to 3 decimal places.
- Saved the final file as "986840_v1_soapi_doc_and_cdom.csv".

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Related Publications

A. Aminot; F. Rey. (2001). Chlorophyll a: Determination by spectroscopic methods. ICES. https://doi.org/10.17895/ICES.PUB.5080 https://doi.org/10.17895/ices.pub.5080
Methods

Hudson, J. M., MacDonald, D. J., Estes, E. R., & Luther, G. W. (2019). A durable and inexpensive pump profiler to monitor stratified water columns with high vertical resolution. Talanta, 199, 415–424. doi:10.1016/j.talanta.2019.02.076
Methods

Ohno, T. (2002). Fluorescence Inner-Filtering Correction for Determining the Humification Index of Dissolved

Organic Matter. Environmental Science & Technology, 36(4), 742–746. doi:10.1021/es0155276
Methods

Ouyang, T., McKenna, A. M., & Wozniak, A. S. (2024). Storm-driven hydrological, seasonal, and land use/land cover impact on dissolved organic matter dynamics in a mid-Atlantic, USA coastal plain river system characterized by 21 T FT-ICR mass spectrometry. Frontiers in Environmental Science, 12. https://doi.org/10.3389/fenvs.2024.1379238
Methods

Qian, J., & Mopper, K. (1996). Automated High-Performance, High-Temperature Combustion Total Organic Carbon Analyzer. Analytical Chemistry, 68(18), 3090–3097. https://doi.org/10.1021/ac960370z
Methods

Wozniak, A. S., Bauer, J. E., & Dickhut, R. M. (2012). Characteristics of water-soluble organic carbon associated with aerosol particles in the eastern United States. Atmospheric Environment, 46, 181–188. https://doi.org/10.1016/j.atmosenv.2011.10.001
Methods

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Parameters

Parameter	Description	Units
Cruise	Cruise name. SOAPI1 = Summer 2022 cruise; SOAPI2 = Fall 2022 cruise; SOAPI3 = Summer 2024 cruise.	unitless
Cruise_ID	Cruise identifier	unitless
Sample_Number	Sample ID number	unitless
Station_and_Day	Station and Day ID, with "S#" denoting the station number and the accompanying letter indicating the sampling day at that station during the cruise.	unitless
Station	The station names are Virginia Coast, Delaware Coast, Continental Slope, and Open Ocean.	unitless
ISO_DateTime_UTC	Station timestamp (UTC) in ISO 8601 format	unitless
Time_of_Day	Time of the day during sample collection (afternoon, evening, morning, night)	unitless
Type	Sample type where ML = sea surface microlayer sample and SS = subsurface seawater sample	unitless
Latitude	Station latitude, south is negative	decimal degrees
Longitude	Station longitude, west is negative	decimal degrees

Salinity	Surface seawater salinity during sample collection	practical salinity units
Surface_Temp	Surface seawater temperature during sample collection	degrees Celsius
Air_Temperature	Air temperature during sample collection	degrees Celsius
Humidity	Humidity during sample collection	percent
WindSpeed_knots	Windspeed during sample collection in knots	knots
Windspeed_m_s	Windspeed during sample collection in meters per second	meters per second (m s-1)
Chlorophyll_a	Chlorophyll-a concentration	microgram per liter (ug L-1)
DOC_uM	Dissolved organic carbon concentration (micromolar)	micromolar (uM)
DOC_mg_L	Dissolved organic carbon concentration (milligrams per liter)	milligram per liter (mg L-1)
BIX	Biological Index from FDOM analysis	unitless
FI	Fluorescence Index from FDOM analysis	unitless
HIX	Humification Index from FDOM analysis	unitless
a254	Napierian absorption coefficient at 254nm	per meter (m-1)
a300	Napierian absorption coefficient at 300nm	per meter (m-1)
S275_295	Spectral slope of wavelength region (275–295 nm)	per nanometer (nm -1)
SR	Slope ratio	unitless
SUVA254	Specific UV absorbance at 254nm	liters per milligram of carbon per meter (L mg-C-1)

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Instruments

Dataset-specific Instrument Name	modified pump profiler system
Generic Instrument Name	CTD - profiler
Dataset-specific Description	Subsurface seawater (SSW) was collected from the starboard side of the ship using a modified pump profiler system (Hudson et al. 2019). The system permits the collection of ~15 L of water in one minute without exposure to O2 from air for discrete sampling of chemical, microbial and other constituents as well as for real time analyses using sensors.
Generic Instrument Description	The Conductivity, Temperature, Depth (CTD) unit is an integrated instrument package designed to measure the conductivity, temperature, and pressure (depth) of the water column. The instrument is lowered via cable through the water column. It permits scientists to observe the physical properties in real-time via a conducting cable, which is typically connected to a CTD to a deck unit and computer on a ship. The CTD is often configured with additional optional sensors including fluorometers, transmissometers and/or radiometers. It is often combined with a Rosette of water sampling bottles (e.g. Niskin, GO-FLO) for collecting discrete water samples during the cast. This term applies to profiling CTDs. For fixed CTDs, see https://www.bco-dmo.org/instrument/869934.

Dataset-specific Instrument Name	Horiba Aqualog spectrofluorometer
Generic Instrument Name	Horiba Aqualog spectrofluorometer
Dataset-specific Description	Fluorescence spectra were collected using a Horiba Aqualog spectrofluorometer.
Generic Instrument Description	A benchtop optical spectrometer suitable for measuring coloured dissolved organic matter (CDOM). Outputs include absorbance spectra, fluorescence emission spectra, and fluorescence excitation-emission matrices. This instrument simultaneously measures absorbance spectra and fluorescence Excitation-Emission Matrices. It employs the Absorbance-Transmission Excitation Emission Matrix (A-TEEM) technique to acquire an Excitation Emission Matrix.

Dataset-specific Instrument Name	RM Young 26700
Generic Instrument Name	Meteorological Station
Dataset-specific Description	Wind velocity and air temperature were measured and recorded continuously with the ship’s meteorological station (RM Young 26700).
Generic Instrument Description	MET station systems are designed to record meteorological information on board ships or mounted on moorings. These are commonly referred to as EMET (Electronic Meteorological Packages) or IMET (Improved Meteorological Packages) systems. These sensor packages record measurements of sea surface temperature and salinity, air temperature, wind speed and direction, barometric pressure, solar and long-wave radiation, humidity and precipitation.

Dataset-specific Instrument Name	SBE 45, Sea-Bird
Generic Instrument Name	Sea-Bird SBE 45 MicroTSG Thermosalinograph
Dataset-specific Description	Sea surface temperature and salinity were measured and recorded continuously with the shipboard instrumentation (SBE 45, Sea-Bird, at 3.7 m depth).
Generic Instrument Description	A small externally powered, high-accuracy instrument, designed for shipboard determination of sea surface (pumped-water) conductivity and temperature. It is constructed of plastic and titanium to ensure long life with minimum maintenance. It may optionally be interfaced to an external SBE 38 hull temperature sensor. Sea Bird SBE 45 MicroTSG (Thermosalinograph)

Dataset-specific Instrument Name	Shimadzu TOC-V
Generic Instrument Name	Shimadzu TOC-V Analyzer
Dataset-specific Description	Used to quantify DOC concentrations.
Generic Instrument Description	A Shimadzu TOC-V Analyzer measures DOC by high temperature combustion method.

Dataset-specific Instrument Name	AU10, Turner
Generic Instrument Name	Turner Designs Fluorometer 10-AU
Dataset-specific Description	Chlorophyll a concentrations were continuously measured with the shipboard fluorometer (AU10, Turner).
Generic Instrument Description	The Turner Designs 10-AU Field Fluorometer is used to measure Chlorophyll fluorescence. The 10AU Fluorometer can be set up for continuous-flow monitoring or discrete sample analyses. A variety of compounds can be measured using application-specific optical filters available from the manufacturer (read more from Turner Designs, turnerdesigns.com, Sunnyvale, CA, USA).

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Deployments

HRS2213

Website	https://www.bco-dmo.org/deployment/990301
Platform	R/V Hugh R. Sharp
Start Date	2022-08-29
End Date	2022-09-03
Description	See more information from R2R: https://www.rvdata.us/search/cruise/HRS2213

HRS2215

Website	https://www.bco-dmo.org/deployment/990303
Platform	R/V Hugh R. Sharp
Start Date	2022-11-09
End Date	2022-11-11
Description	See more information at R2R: https://www.rvdata.us/search/cruise/HRS2215

HRS2407

Website	https://www.bco-dmo.org/deployment/990307
Platform	R/V Hugh R. Sharp
Start Date	2024-08-11
End Date	2024-08-21
Description	See more information at R2R: https://www.rvdata.us/search/cruise/HRS2407

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Project Information

Collaborative Research: Impacts of surface ocean surfactant sources and transformations on their chemical composition and air-sea relevant properties (SOAPI)

Coverage: Western North Atlantic surface waters

NSF abstract:
The surface microlayer (SML), the thin layer of water at the interface between the ocean and the atmosphere, controls the exchange of materials to and from the ocean. As a result, it can profoundly influence biogeochemical cycles and global climate. One type of chemical species that accumulates at this interface are surfactant molecules, which influence the surface tension of and the rate of material exchange at air-water interfaces. Biological and chemical production and degradation processes represent surfactant sources and removal pathways, but the relative importance of those processes for determining surfactant quantities and molecular composition remains unclear. Similarly, the relationship between surfactant molecule composition and surface tension at the air-water interface has not been established. As a result, their effects on material exchange at the interface cannot currently be predicted. This work will use measurements at sea, laboratory experiments, and high-resolution analyses to measure the chemical and physical characteristics of surfactants and their properties at the air-sea interface. An improved understanding of surfactant processes and surface ocean will benefit society by improving our understanding of the exchange of climate-relevant gases and particles. Two early career PIs will advance their established collaboration and gain further experience leading research projects and mentoring students. Students will receive valuable hands-on training in oceanographic field collections, state-of-the-science analytical techniques, data interpretation, and data dissemination. The results and methodologies from this work will be featured in courses at the University of Georgia and the University of Delaware and will be developed into content for K-12 students, enhancing infrastructure for education.

This work includes the unique pairing of state-of-the-science measurements across time and spatial scales to assess the influence of oceanographic processes on surfactant chemical composition and physical air-sea relevant properties. SML and subsurface waters will be collected from estuarine, coastal ocean, and open ocean sites during high and low productivity conditions to establish surfactant molecular characteristics over a range of space, time, and ocean biological activity. The effects of light will be assessed via diurnal sampling efforts and laboratory experiments. Samples will be analyzed for their detailed chemical, biological, and physical characteristics. The surface tension of the SML is expected to be inversely correlated with the abundance of lipid-like compounds (low O content, high H/C ratios, e.g., sulfur-containing lipids) produced during periods of high biological activity. Prolonged exposure to light is hypothesized to result in photo-oxidation of surfactant compounds, higher abundances of oxygenated and lower molecular weight aliphatic compounds, and increased surface tension. Multivariate statistical approaches will be used to reveal a mechanistic understanding of the links between biological and photochemical processes and the resulting surfactant and SML chemical and physical characteristics. This new knowledge will represent a first step toward improved models of the air-sea exchange of climate relevant gases which currently have large uncertainties. It will inform future work on the exchange of volatile and aerosol organics with significant potential impacts for our understanding of the climate system.

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-2123402
NSF Division of Ocean Sciences (NSF OCE)	OCE-2123368

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