Mercury, methylmercury, nutrients, and physicochemical measurements from water column samples collected in the Gulf of Maine and Penobscot Estuary during several cruises in 2023 and 2024

Website: https://www.bco-dmo.org/dataset/990899
Data Type: Cruise Results
Version: 1
Version Date: 2026-01-12

Project
» Collaborative Research: The effects of terrestrial organic matter inputs on coastal mercury cycling, methylmercury production and bioaccumulation (Mercury in the Gulf of Maine)

Contributors	Affiliation	Role
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Abstract
This dataset includes water chemistry data from Gulf of Maine (GoM) cruises in April, August, and November 2023, and April 2024, as well as from two trips to the Penobscot River and Estuary in August 2023 and April 2024. This includes mercury (Hg), methylmercury (MeHg) in the water column, nutrients, and physicochemical data.

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Coverage

Location: Gulf of Maine and Penobscot Estuary
Spatial Extent: **N**:44.60633 **E**:-66.43346 **S**:43.4715 **W**:-69.7678
Temporal Extent: 2023-04-04 - 2024-05-07

Methods & Sampling

Description:
Total mercury, methylmercury, and ancillary variable data were collected in the Gulf of Maine along the Gulf of Maine North Atlantic Time Series (GNATS) transect and on a transect in the Penobscot Estuary and River. Sampling took place over four cruises on the R/V Endeavor (April 2023, August 2023, November 2023, April 2024), and two separate trips in a small boat to sample further upstream in the Penobscot River (September 2023, May 2024). 21 stations were sampled in total, with multiple depths (up to 6) extending throughout the water column at all stations except for the shallow Penobscot River stations.

This dataset includes bulk and particulate total mercury and monomethylmercury, dissolved organic carbon, particulate organic carbon and nitrogen, chlorophyll-a, phaeopigments, nitrate, phosphate, silicate, fluorescence indices (including the freshness index, BIX, and HIX), and components identified during Parallel Factor (PARAFAC) analysis. The percentage of methylated mercury (bulk methylmercury/bulk total mercury), percentage of particulate methylated mercury (particulate methylmercury/particulate total mercury), and percentage of each PARAFAC component are also included. The dataset also includes salinity, temperature, and dissolved oxygen data from the sensors on the CTD, as well as the calculated apparent oxygen utilization. Nutrient data in August in the Gulf of Maine was replaced with data supplied by DFO from a transect similar to the GNATS transect, which occurred in September 2023.

Methods & Sampling:
During the four cruises, samples were collected using a trace metal clean rosette with Go-Flo bottles. During the August 2023 cruise, the trace metal clean rosette and winch system suffered a technical issue that was unable to be resolved, thus Stations 3, 4, 6, 7, and 10-15 were collected with the same Go-Flo bottles attached to a non-trace metal clean, Seabird rosette. Water samples were collected over the side of a small watercraft for the Penobscot River sites, taken either by hand or via Go-Flo bottles. Bulk water samples were collected in 2-liter (L) acid-cleaned Teflon bottles and then brought into a trace metal clean van (or laminar flow hood for the Penobscot River sites) for typically immediate, but if not same-day, filtering and subsampling.

Bulk Methylmercury samples were preserved with sulfuric acid (0.5%) and kept cold until analysis. They were analyzed on a Tekran 2700 Automated Methylmercury Analysis System following standard techniques (Hammerschmidt and Fitzgerald, 2006). Briefly, bulk MeHg samples were digested overnight with sulfuric acid, buffered with acetate buffer, followed by the addition of ascorbic acid, neutralized with potassium hydroxide, and ethylated using sodium tetraethylborate. Once on the Tekran 2700, samples were purged with argon, and the Hg species were trapped on a Tenax trap. Upon heating the trap, the Hg species were released and underwent gas chromatographic separation prior to decomposition of the Hg species to elemental Hg for cold vapor atomic fluorescence detection. Samples were run within 6 months of collection at the University of Connecticut Avery Point.

Particulate methylmercury was filtered through a pre-weighed and pre-combusted (400 degrees Celsius (°C), 15-18 hours), 0.45-micrometer (µm) pore-size, quartz fiber filter using a vacuum pump and frozen until analysis. Filters were freeze-dried for 7 days, weighed, and then digested in 4.5 N nitric acid overnight in a 60°C water bath, buffered with acetate buffer, neutralized with potassium hydroxide, and ethylated using sodium tetraethylborate, where the sample then underwent the same process on the Tekran 2700 as described above. The remaining digest - 3 milliliters (mL) out of 7 mL total - was frozen and preserved within 1 week for THg analysis by diluting to 10 mL with DI water, adding bromine monochloride, and storing in the dark at room temperature. Filters were run within 1 year of collection at the University of Connecticut Avery Point.

Bulk total mercury samples were filled with no headspace and kept cold until analysis on a Tekran 2600 following EPA method 1631, refined by Hammerschmidt and Fitzgerald (2006). Briefly, both particulate and bulk samples were digested overnight with bromine chloride, reduced with hydroxylamine hydrochloride to remove excess reductant, oxidized with stannous chloride to form elemental Hg, and run using cold vapor atomic fluorescence spectrometry. Samples were run within 6 months of collection at the University of Connecticut Avery Point.

Particulate total mercury was analyzed using the same filter as for particulate methylmercury and run using the method described above. Filters were run within 1 year of collection at the University of Connecticut Avery Point.

Chlorophyll-a and phaeopigments were collected by filtering 100 mL of sample through a 25-millimeter (mm), 0.7 µm pore-size glass fiber filter using a vacuum pump and immediately covering with tin foil and freezing. The filters were pre-combusted (450°C, 2 hours) for the April 2024 cruise and 2024 Penobscot river samples only. Samples were analyzed using EPA method 445. Briefly, the filters were digested overnight in 90% acetone and run in dimmed light with and without hydrochloric acid acidification using a Trilogy Fluorometer. Samples were only collected for the shallowest 3 to 4 depths at each station for all cruises except April 2023 because the chlorophyll-a was found to be below the limit of detection (LOD) at depth during the April 2023 cruise. The bottom depths for chlorophyll-a were replaced with ½ the LOD, based on the CTD fluorescence scans, which confirmed the lack of chlorophyll-a at depth. Phaeopigment data at depth were left blank due to inability to confirm or deny the lack of phaeopigments at depth. Chlorophyll and phaeopigment concentrations were calculated using equations based on the EPA method 445. Some phaeopigment values came back negative; these samples were assumed to contain no phaeopigments. Samples were run within 1 month of collection, except for in April 2023 where they were run within 3 months of collection at the University of Connecticut Avery Point.

Particulate organic carbon and nitrogen samples were collected by filtering 200 mL (300 mL in November 2023) of sample through a 25 mm, 0.7 µm pore-size, pre-combusted (450°C, 2 hours) glass fiber filter using a vacuum pump and immediately covering with tin foil and freezing. POC/N filters were saturated with hydrochloric acid for 4 to 12 hours, allowed to dry overnight in the hood, and dried at 45°C for at least 3 days in the oven. Filters were weighed and re-dried for a couple of hours to ensure the drying process was complete and kept in a sealed desiccator until analysis (within 1 year of collection). Samples were run on a Fisons NA 1500 series 2 elemental analyzer by Costech Analytical Technologies using procedures based on the EPA method 440. Several samples did not have any peaks associated with nitrogen; these samples were replaced with ½ the LOD. Samples were processed within 14 months of collection at the University of Connecticut Avery Point.

Dissolved organic carbon samples were filtered through a 25 mm, 0.7 µm pore-size, pre-combusted (450°C, 2 hours) glass fiber filter and were frozen until analysis. Samples were acidified to 0.5% with hydrochloric acid and analyzed with a Shimadzu TOC analyzer within seven months of collection at the University of Connecticut Avery Point.

Nitrate, phosphate, and silicate samples were filtered through a 25 mm, 0.7 µm pore-size glass fiber filter and were frozen until analysis. Filters were pre-combusted (450°C, 2 hours) for the April 2024 cruise and Penobscot river trip only. Samples were analyzed via standard colorimetric methods using a Shimazdu UV-1900i Spectrophotometer (Hansen & Koroleff, 1999). Samples were analyzed within approximately one year of collection at Dartmouth College. Results from April 2023 and August were not included due to concerns about data quality. August data was replaced with data from a cruise by DFO from September 27th to the 29th, 2023, which followed a transect close to the GNATS transect (Figure S1). Data was substituted if it was collected from within 15 meters of this study's depths.

Dissolved organic matter samples were filtered through a 25 mm, 0.7 µm pore-size, pre-combusted (450°C, 2 hours) glass fiber filter and were frozen until analysis (they were defrosted for short periods to obtain a subsample for DOC analysis). Samples were run using a Cary Eclipse Fluorescence Spectrophotometer (excitation: 220-550 nanometer (nm), emission: 300-700 nm, slit width: 5 nm, increment by 5 nm, PMT voltage: 800, scan speed: 900 nm/minute) within 14 months of collection at the University of Connecticut Avery Point. Absorbance scans were run using a Shimazdu UV-1900i Spectrophotometer from a wavelength of 200 to 700 nm within 18 months of collection at Dartmouth College. Only samples from the upper 30 meters of the water column were analyzed. Data was processed by Urban Wünsch (Technical University of Denmark) using Parallel Factor (PARAFAC) analysis to obtain fluorescence indices and PARAFAC components.

Salinity, temperature, and dissolved oxygen were collected using either the CTD or a hand-held Sonde (for the Penobscot River sites).

Apparent Oxygen Utilization was calculated using the equation and constants from Garcia & Gordon (1992).

Hg data was blank and spike corrected and ancillary variables were blank-subtracted, with the exception of the nutrient data. THg and MeHg bulk samples were run in triplicate. For the other variables, triplicate samples were collected at varying stations and depths throughout the cruises. Any data below the limit of detection (LOD) was replaced with the LOD. The LOD was defined as 3 times the standard deviation of the blanks. A table with the average QA/QC parameters is included (Table 1, see Supplemental File, "990899_v1_Table_1.pdf").

BCO-DMO Processing Description

- Imported original file "GoM_Penobscot_Data.xlsx" into the BCO-DMO system.
- Marked "NaN" and "nd" as missing data identifiers (missing data are empty/blank in the final CSV file).
- Replaced "15:37.30" with "15:37:30" in the Date_Time_UTC column.
- Converted the Date_Time_UTC column to ISO 8601 format.
- Saved the final file as "990899_v1_gulf_of_maine_hg.csv".

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Related Publications

Arar, E. J. & Collins, G. B. (1997). In vitro determination of chlorophyll a and phaeophtin a in marine and freshwater phytoplankton by fluorescence – USEPA Method 445.0. Revision 1.2. In: USEPA methods for determination of chemical substances in marine and estuarine environmental samples. Cincinnati, OH. URL: https://cfpub.epa.gov/si/si_public_record_report.cfm?Lab=NERL&dirEntryId=309417
Methods

Garcia, H. E., & Gordon, L. I. (1992). Oxygen solubility in seawater: Better fitting equations. Limnology and Oceanography, 37(6), 1307–1312. doi:10.4319/lo.1992.37.6.1307
Methods

Hammerschmidt, C. R., & Fitzgerald, W. F. (2006). Bioaccumulation and Trophic Transfer of Methylmercury in Long Island Sound. Archives of Environmental Contamination and Toxicology, 51(3), 416–424. doi:10.1007/s00244-005-0265-7
Methods

Hansen, H. P., & Koroleff, F. (1999). Determination of nutrients. In Methods of Seawater Analysis (pp. 159–228). Wiley. https://doi.org/10.1002/9783527613984.ch10
Methods

U.S. Environmental Protection Agency. Method 1631, Revision E: Mercury in Water by Oxidation, Purge and Trap, and Cold Vapor Atomic Fluorescence Spectrometry Method 1631, Revision E: Washington, D.C., 2002. https://www.epa.gov/sites/default/files/2015-08/documents/method_1631e_2002.pdf
Methods

Zimmerman, C. F., C. W. Keefe, & J. Bashe. (1997). Method 440.0 Determination of Carbon and Nitrogen in Sediments and Particulatesof Estuarine/Coastal Waters Using Elemental Analysis. U.S. Environmental Protection Agency, Washington, DC, EPA/600/R-15/009.
Methods

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Parameters

Parameter	Description	Units
Cruise_ID	Official cruise identifier. I.e. EN699 = R/V Endeavor cruise number 699. "NA" represents samples taken from a small boat, not the R/V Endeavor.	unitless
Cruise_Name	Month and year of the cruise. This is how the cruise is referenced in the publication.	unitless
Date_Time_UTC	Date and time (UTC) when the CTD was deployed for each station.	unitless
Latitude_N	Latitude of the sample station.	decimal degrees
Longitude_W	Longitude of the sample station.	decimal degrees
WaterColumn_Depth	Depth of the seafloor at each station.	meters (m)
Station_Num	Station number.	unitless

Sample_ID	Identifying number for each sample. The first digits are the station number, followed by two zeros, followed by the position in the water column. 1 represents surface samples, and 6 represents the deepest sample. Ex: 7002 represents station 7, the 2nd sample from the surface. Samples with a "P" at the end were collected in the Penobscot River, not during the R/V Endeavor cruises.	unitless
Sample_Depth_m	Depth that the sample was collected.	meters (m)
Temp	Water temperature.	Degrees Celsius (°C)
Salinity	Salinity of water.	Pratical Salinity Units (psu)
Oxygen	Concentration of dissolved oxygen in the water.	micromoles per kilogram (µmol/kg)
AOU	Calculated apparent oxygen utilization in the water.	micromoles per kilogram (µmol/kg)
Bulk_THg	Unfiltered concentration of total mercury in water.	picomoles (pM)
pTHg	Particulate total mercury in water.	picomoles (pM)
Bulk_MeHg	Unfiltered concentration of methylmercury in water.	picomoles (pM)
pMeHg	Particulate methylmercury in water.	picomoles (pM)
Percent_MeHg	Percentage of bulk methylmercury in bulk total mercury. I.e. Bulk_MeHg/Bulk_THg.	unitless (percent)
Percent_pMeHg	Percentage of particulate methylmercury in particulate total mercury. I.e. pMeHg/pTHg.	unitless (percent)
DOC	Dissolved organic carbon in water.	micromolar (µM)
PON	Particulate organic nitrogen in water.	micrograms per Liter (µg/L)
POC	Particulate organic carbon in water.	micrograms per Liter (µg/L)
Chl_a	Chlorophyll-a in water.	micrograms per Liter (µg/L)

Pha	Phaeopigments in water.	micrograms per Liter (µg/L)
NOx	Nitrate and nitrite in water.	micromolar (µM)
PO4	Phosphate in water.	micromolar (µM)
SiO4	Silicate in water.	micromolar (µM)
Freshness_Index	Freshness Index.	unitless
BIX	Biological Index.	unitless
HIX	Humification Index.	unitless
PercentC1	Percentage of PARAFAC component 1. I.e. C1/Sum of all components.	unitless (percent)
PercentC2	Percentage of PARAFAC component 2. I.e. C2/Sum of all components.	Percentage
PercentC3	Percentage of PARAFAC component 3. I.e. C3/Sum of all components.	Percentage
PercentC4	Percentage of PARAFAC component 4. I.e. C4/Sum of all components.	Percentage
PercentC5	Percentage of PARAFAC component 5. I.e. C5/Sum of all components.	Percentage
PercentC6	Percentage of PARAFAC component 6. I.e. C6/Sum of all components.	Percentage
C1	PARAFAC component 1.	unitless
C2	PARAFAC component 2.	unitless
C3	PARAFAC component 3.	unitless
C4	PARAFAC component 4.	unitless
C5	PARAFAC component 5.	unitless
C6	PARAFAC component 6.	unitless

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Instruments

Dataset-specific Instrument Name	Fisons NA 1500 series 2 elemental analyzer
Generic Instrument Name	Elemental Analyzer
Dataset-specific Description	Used to measure particulate organic carbon and nitrogen.
Generic Instrument Description	Instruments that quantify carbon, nitrogen and sometimes other elements by combusting the sample at very high temperature and assaying the resulting gaseous oxides. Usually used for samples including organic material.

Dataset-specific Instrument Name	Go-Flo bottles
Generic Instrument Name	GO-FLO Bottle
Generic Instrument Description	GO-FLO bottle cast used to collect water samples for pigment, nutrient, plankton, etc. The GO-FLO sampling bottle is specially designed to avoid sample contamination at the surface, internal spring contamination, loss of sample on deck (internal seals), and exchange of water from different depths.

Dataset-specific Instrument Name	Cary Eclipse Fluorescence Spectrophotometer
Generic Instrument Name	Spectrophotometer
Dataset-specific Description	Produced excitation emission matrixes for dissolved organic matter.
Generic Instrument Description	An instrument used to measure the relative absorption of electromagnetic radiation of different wavelengths in the near infra-red, visible and ultraviolet wavebands by samples.

Dataset-specific Instrument Name	Tekran 2600 cold vapor atomic fluorescence spectrometer
Generic Instrument Name	Tekran 2600 Automated Total Mercury Analyzer series
Dataset-specific Description	Used to measure bulk and particulate total mercury.
Generic Instrument Description	The Tekran 2600 is a total Mercury (Hg) analysis system that can measure sub-picogram quantities of mercury in water, soil, vegetation, and other sample matrices. The system utilizes a Cold Vapour Atomic Fluorescence Spectroscopy (CVAFS) detector. The 2600-IVS (In-Vial Sparging) model is reconfigured for direct in-vial sparging sample introduction, and the 2600-NG (Natural Gas) model is designed for the analysis of gas phase sample cartridges. The system is capable of multiple method configurations: Dual stage gold preconcentration (EPA Method 1631); Direct measurement without preconcentration (EPA Method 245.7); Air sample analysis on gold traps (EPA Compendium Method IO-5); and Natural gas analysis on gold traps (ASTM D-6350, ISO 6978). It has a guaranteed minimum detection limit of < 0.05 nanograms per liter (ng/L). In clean room environments, with low mercury blanks, minimum detection limits as low as 0.02 ng/L are achievable. See: https://www.tekran.com/products/laboratory/tekran-model-2600-automated-t...

Dataset-specific Instrument Name	Tekran 2700 Automated Methylmercury Analysis System
Generic Instrument Name	Tekran Model 2700 Automated Methyl Mercury Analysis System
Dataset-specific Description	Used to measure bulk and particulate methylmercury samples. The instrument incorporates gas chromatography and cold vapor atomic fluorescence detection.
Generic Instrument Description	The Tekran 2700 is a fully integrated Gas Chromatography Cold-Vapor Atomic Fluorescence Spectrophotometer (GC-CVAFS) automated Methyl Mercury analysis system. The 2700 can analyze distilled waters, extracted or distilled tissues and solids, and allows direct analysis of suitable water samples. The system is pre-programmed to run EPA Method 1630, however it offers complete method customization including: GC column temperature ramping; programmable analysis cycle settings; high temperature purge cycles; and choice of trap and GC column. It can also interface with ICP-MS or other analytical instruments. The sample analysis cycle is less than 7 minutes per sample. It has a minimum detection limit of 0.002 nanograms per liter (ng/L). The system has IR trap heating and active cooling. See: https://www.tekran.com/products/laboratory/tekran-model-2700-automated-m...

Dataset-specific Instrument Name	Shimadzu TOC analyzer
Generic Instrument Name	Total Organic Carbon Analyzer
Dataset-specific Description	Used to measure dissolved organic carbon.
Generic Instrument Description	A unit that accurately determines the carbon concentrations of organic compounds typically by detecting and measuring its combustion product (CO2). See description document at: http://bcodata.whoi.edu/LaurentianGreatLakes_Chemistry/bs116.pdf

Dataset-specific Instrument Name	Trilogy Fluorometer
Generic Instrument Name	Turner Designs Trilogy fluorometer
Dataset-specific Description	Used to measure chlorophyll-a and phaeopigments.
Generic Instrument Description	The Trilogy Laboratory Fluorometer is a compact laboratory instrument for making fluorescence, absorbance, and turbidity measurements using the appropriate snap-in application module. Fluorescence modules are available for discrete sample measurements of various fluorescent materials including chlorophyll (in vivo and extracted), rhodamine, fluorescein, cyanobacteria pigments, ammonium, CDOM, optical brighteners, and other fluorescent compounds.

Dataset-specific Instrument Name	Shimazdu UV-1900i Spectrophotometer
Generic Instrument Name	UV Spectrophotometer-Shimadzu
Dataset-specific Description	Used to measure nitrate, inorganic phosphate, and silicate. Also used to measure dissolved organic matter fluorescence.
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: The effects of terrestrial organic matter inputs on coastal mercury cycling, methylmercury production and bioaccumulation (Mercury in the Gulf of Maine)

Coverage: Gulf of Maine and the Penobscot River estuary

NSF Award Abstract:
Climate change will influence the delivery of contaminants, organic matter, and nutrients from land to the coastal ocean. This is because higher rainfall and warming increase runoff from land to coastal waters. Runoff also influences coastal algal blooms. These changes are expected to alter the distribution of mercury in the water and impact its availability for biological uptake. Mercury is a potent toxin. Its uptake into the food web contaminates fish and seafood and affects human health. This project will study how organic matter delivered from land to coastal waters affects mercury concentrations in seawater and in the food webs of the Gulf of Maine. The Gulf of Maine is one of the largest and most important coastal fishing grounds in the United States. This project will measure the concentration and isotopes of mercury on samples collected from research cruises under different algal bloom conditions and river flows. Lab experiments will be used to study how land-derived organic matter affects mercury accumulation in plankton. The project will provide research experiences for four undergraduate students in a STEM field. Training will be provided to a PhD student and a postdoctoral fellow. Findings from the project will provide critical information about the effect of climate change on mercury levels in marine waters and food webs. This information is needed for achieving the goals of the Minamata Convention, a global treaty for reducing mercury emissions to the environment.

This project will examine the effects of climate change on terrestrial organic matter and mercury concentrations in Gulf of Maine waters. Specifically, the scientists will study the complex and often competing processes that influence: 1) mercury cycling and distribution; 2) the formation of methylmercury; and 3) methylmercury uptake to microplankton. Terrestrial organic matter plays an important role in transferring mercury from watersheds to coastal and offshore waters. It also controls the formation of methylmercury in water by providing a microenvironment that promotes the methylation of mercury by microbes, which represents the first step for uptake of methylmercury into seafood. However, some plankton can directly use organic matter as a food source (so-called “mixotrophs”) and can bioaccumulate methylmercury during feeding. Mixotrophs can dominate microplankton assemblages in coastal waters at some times of the year, and previous studies have not explored the impact of this feeding mode on methylmercury uptake at the base of the food web. This project will study the effects of organic matter dynamics on mercury and methylmercury cycling and bioaccumulation through 1) field surveys and shipboard experiments in the Gulf of Maine, where delivery of terrestrial organic matter is increasing, and 2) through laboratory microcosm experiments using autotrophic and mixotrophic microplankton taxa under contrasting carbon acquisition modes and organic matter characteristics and concentrations. This work will also apply novel mercury and methylmercury-specific isotope analyses and measures of organic matter quality to increase understanding of mercury cycling in coastal environments. This research will fill important gaps in predicting the effects of environmental changes on marine methylmercury levels, providing critical information to mitigating mercury emissions and methylmercury exposures, and for predicting changes in mercury levels in seafood in the future.

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-2148407
NSF Division of Ocean Sciences (NSF OCE)	OCE-2148683

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