Dissolved organic matter (DOM) optical properties in surface waters of the Upper Newport Back Bay estuary in California from May 2021 to July 2022

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Project
» RUI: Collaborative Research: Cycling of ethanol and acetaldyhyde in coastal waters (Coastal Water Cycling)

Contributors	Affiliation	Role
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Abstract
These data are measurements of the optical properties of dissolved organic matter (DOM) in near-shore surface waters of the Upper Newport Back Bay estuary in Southern California in 77 samples taken between May 2021 and July 2022. The optical properties were measured to characterize DOM associated with the photochemical production of ethanol and acetaldehyde in estuarine waters. The goal of this project was to improve understanding of the cycling of the atmospheric pollutants ethanol and acetaldehyde in coastal seawater and surface waters. These data were collected by Dr. Warren De Bruyn of Chapman University.

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Coverage

Location: Newport Back Bay (NBB) estuary in Orange County, Southern California, USA
Spatial Extent: **N**:33.650327 **E**:-117.8671967 **S**:33.6181867 **W**:-117.9051099
Temporal Extent: 2021-05-20 - 2022-07-13

Methods & Sampling

The Newport Back Bay (NBB) is an estuary in Orange County, Southern California, USA. It includes the Upper Newport Back Bay, a ~1000-acre ecological preserve managed by the U.S. Fish and Wildlife Service and the California Department of Fish and Game. This estuary includes salt marshes and mudflats. The primary freshwater input is the San Diego creek which drains a ~150 square mile watershed, with additional freshwater inputs from some storm-water drains. Water samples were collected from 3 sites: Site 1 (inlet; 33.650327, -117.8671967); site 2 (mid-estuary; 33.6302266, -117.8859726); site 3 (near the outlet into the Pacific Ocean; 33.6181867, -117.9051099). When freshwater inflow is significant, site 1 has lower salinity water with higher dissolved organic content.

Surface water (<5 cm) was sampled in the morning from the shore, stored in amber glass bottles, transported

to the laboratory, filtered through 0.2 micron Durapore filters and stored in the fridge. Optical properties were measured to assess the dissolved organic content of the sample and allow for the estimation of the photochemical production rates of ethanol and acetaldehyde. Samples were filtered through 0.2 micron Durapore filters to remove microorganisms. Spectra were obtained in a 1 cm quartz cell using a Horiba Aqualog spectrofluorometer. Excitation-emission matrices (EEMs) were also collected (excitation 250-450 nm; emission 250 to 830 nm). Nanopure water was used as the blank. EEMs were corrected for inner filter effects and 1st order Rayleigh scattering using post-measurement routines of the Aqualog. Raw absorbance data were used to calculate absorption coefficients.

These methods are described in more detail in Juetten et al. (2025).

Data Processing Description

The maximum fluorescence intensity associated with terrestrial humic-like peaks A and C and protein-like peak T in the measured EEMs were recorded. The EEMs were used to calculate several optical indices. The fluorescence index (FIX) is the ratio of emission at 450 nm to emission at 500 nm for an excitation of 370 nm. FIX is about 1.3 for allochthonous terrestrial and soil material and higher at ~1.9 for autochthonous aquatic and microbial sources. The humification index (HIX) is the ratio of integrated emission intensities from 435 – 480 nm and 300 – 345 nm at 254 nm excitation. More aromatic, humified terrestrial material typically has higher HIX values . The index of recent autochthonous contribution (BIX) is the ratio of emission intensities at 380 and 430 nm for an excitation of 310 nm. BIX < 0.6 have been associated with terrestrial DOM sources and BIX >1 have been attributed to autochthonous inputs. This is summarized from Juetten et al. (2025).

BCO-DMO Processing Description

* added lat/lon of each sampling site to dataset
* converted date to ISO format

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Related Publications

Juetten, K., De Bruyn, W. J., Landram, Z., Jansen, C. D. R., Harrison, A. W., Strecker, A., & Clark, C. D. (2025). Production of dissolved organic matter from lily pads (Nymphaea odorata) in a mesotrophic freshwater lake. Aquatic Sciences, 87(2). https://doi.org/10.1007/s00027-025-01180-4
Methods

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Parameters

Parameter	Description	Units
date	date sample taken	unitless
site	location sample was taken	unitless
latitude	sampling latitude, south is negative	decimal degrees
longitude	sampling longitude, west is negative	decimal degrees
BIX	index of recent autochthonous contribution	unitless
HIX	humification index	unitless
FIX	fluorescence index	unitless
Flu	fluorescence intensity at an excitation of 350 nm and emission of 450 nm	millivolts (mV)
A	intensity of humic-like peak A	millivolts (mV)
C	intensity of humic-like peak C	millivolts (mV)
T	intensity of humic-like peak T	millivolts (mV)

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Instruments

Dataset-specific Instrument Name	Horiba Aqualog
Generic Instrument Name	Spectrometer
Dataset-specific Description	Horiba Aqualog spectrometer was used to measure optical properties of DOM
Generic Instrument Description	A spectrometer is an optical instrument used to measure properties of light over a specific portion of the electromagnetic spectrum.

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Project Information

RUI: Collaborative Research: Cycling of ethanol and acetaldyhyde in coastal waters (Coastal Water Cycling)

Coverage: Upper Newport Back Bay estuary in Orange County, Southern California

NSF Award Abstract

Ethanol is added to gasoline to increase octane levels and lower the concentrations of carbon monoxide and surface ozone in the atmosphere. As a renewable fuel, ethanol may also help decrease our dependence on gasoline. Increased use of ethanol in the United States and globally as a fossil fuel substitute and additive is expected to increase ethanol levels in the atmosphere. Atmospheric ethanol is converted to acetaldehyde which is a hazardous pollutant. To understand the impact of increasing ethanol usage, it is important to understand the cycling of ethanol and acetaldehyde in the environment--how they are produced, consumed, and interconverted. Because these compounds can cross from air into water, this requires understanding what happens to these compounds in both the atmosphere and in seawater and other surface waters. This proposal focuses on improving our understanding of processes that produce and consume ethanol and acetaldehyde in coastal seawater and other coastal surface waters like estuaries and salt marshes. This project will measure the rates of photochemical production of ethanol and acetaldehyde, as well as their chemical and biological degradation rates. The project will also measure the rate and efficiency of the biological production of acetaldehyde from ethanol by microbial organisms in these waters. The scientists have an excellent track record of involving undergraduate students, including underrepresented minorities, in their research and as co-authors on publications, a trend they plan to continue with this project. These students would be trained in analytical chemistry and environmental research and would present their research findings at local and national conferences. Lastly, the PIs also plan outreach activities with high school STEM programs to improve student diversity in environmental research.

The primary sink for ethanol in the troposphere is reaction with OH to produce acetaldehyde. Acetaldehyde levels in the troposphere are also expected to increase with increased use of ethanol. Changes in the atmospheric concentrations of these species are expected to have a significant impact on the oxidative capacity of the troposphere. To understand future impacts, it is important to understand current tropospheric budgets which have significant uncertainties for both species. One of the largest sources of uncertainty is the role of the oceans and surface waters in cycling these species into and out of the troposphere. The current understanding is limited by the very small database of ambient concentration measurements in both air and water and an incomplete insight into the processes that control concentrations in seawater and surface waters; these processes represent a complex interplay between biological and photochemical sources and sinks, and air-water exchange. To improve the current understanding of the cycling of ethanol and acetaldehyde in coastal seawater and surface waters, this project will measure: 1) chemical and biological degradation rates of ethanol and acetaldehyde in coastal waters; 2) the rate and efficiency of the biological production of acetaldehyde from ethanol by microbial organisms; 3) ethanol and acetaldehyde concentrations in air and surface waters; 4) the ethanol and acetaldehyde source strength of estuary and saltmarsh sediments; and 5) ethanol and acetaldehyde photochemical production rates in surface waters.

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-2022112
NSF Division of Ocean Sciences (NSF OCE)	OCE-2022184

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