

## **Optical and photochemical data of temperate wetland samples collected in Minnesota, USA from 2014-August to 2015-October**

### **Abstract**

Wetland surface water samples were collected from 39 sites throughout Minnesota, USA between 2014-August and 2015-October. Optical and photochemical parameters of the samples were measured under controlled laboratory conditions. The data were collected to identify environmental variables that constrain the yield of triplet excited states of dissolved natural organic matter ( $^3\text{CDOM}^*$ ). Apparent quantum yields ( $\text{AQY}_T$ ) of  $^3\text{CDOM}^*$  were measured using the chemical probe, 2,4,6-trimethylphenol, under a broadband xenon-arc lamp with a 290-nm wavelength filter.

### **General Information**

1. Title of Dataset: Optical and photochemical data of temperate wetland samples collected in Minnesota, USA from 2014-August to 2015-October
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3. Data collected and interpreted: 2014-08 through 2017-10
4. Location of Data Collection:  
University of Minnesota  
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5. Funding sources:

- A. Minnesota Environment and Natural Resources Trust Fund as recommended by the Legislative-Citizen Commission on Minnesota Resources
- B. Doctoral Dissertation Fellowship from the Graduate School at the University of Minnesota
- C. National Science Foundation (CBET-143414)

### **Sharing and Data Access**

1. This work is protected by a Creative Commons Attribution-NonCommercial 4.0 International License.
2. Publication that uses this data:  
McCabe, A. J., and W. A. Arnold (2018), Multiple linear regression models to predict the formation efficiency of triplet excited states of dissolved organic matter in temperate wetlands, *Limnol. Oceanogr.*, <http://dx.doi.org/10.1002/lno.10820>.
3. Suggested citation for this dataset:  
McCabe, A. J., and Arnold, William A. 2017. Optical and photochemical data of temperate wetland samples collected in Minnesota, USA from 2014-August to 2015-October. Retrieved from the Data Repository for the University of Minnesota.

### **Data Overview**

File:

TemperateWetlands\_UofMN\_DataTable.xlsx

Description:

This file contains water chemistry, optical, photochemical, general hydrologic, and spatial data for temperate wetlands sampled from 39 sites in Minnesota, USA collected between 2014-08 through 2015-October.

Missing data code: Missing data are noted by empty cells in the worksheets.

### **Methodological Information**

Description of methods used for data collection:

McCabe, A. J., and W. A. Arnold (2018), Multiple linear regression models to predict the formation efficiency of triplet excited states of dissolved organic matter in temperate wetlands, *Limnol. Oceanogr.*, <http://dx.doi.org/10.1002/lno.10820>.

### **Data-specific information for: TemperateWetlands\_UofMN\_DataTable.xlsx**

1. Worksheet: Water Chem & Photochem

The estimated 95% confidence interval (CI) for each variable is reported in a separate column immediately adjacent to the data. The relative CI (CI/measurement) is also reported as a percentage for select variables. The average standard error of field duplicates is reported as a measure of accuracy for variables that were not quantified from an external calibration curve or from regression of kinetic or experimental data.

Variable List:

A. Name: Site ID

Description: Site identification name.

B. Name: Sample Type

Description: Either 'Sample' or 'Field Duplicate'. Field duplicates were collected at the same time and location as the 'Sample', but in a separate bottle. Eight field duplicates were collected over the duration of the sampling period.

C. Name: Collection Date

Description: Date upon which the sample was collected (DAY-MONTH-YEAR). 'Collection Month' and 'Collection Year' are also given as separate cells.

D. Name: pH

Description:  $\text{pH} = -\log([\text{H}^+])$  [unitless] where  $[\text{H}^+]$  is the concentration of protons [units = M].

E. Name: Specific Conductance

Description: A measure of the samples ability to conduct an electrical current due to the presence of ions in solution. Also, an empirical measure of a sample's ionic strength [units =  $\mu\text{S cm}^{-1}$ ].

F. Name: DOC

Description: DOC is the dissolved organic carbon concentration measured by catalytic combustion [units =  $\text{mg-C L}^{-1}$  and  $\times 10^{-4} \text{ mol-C L}^{-1}$ ].

G. Name: DIC

Description: DIC is the dissolved inorganic carbon concentration measured either by alkalinity titration or off-gassed  $\text{CO}_2$  after sample acidification [units =  $\text{mg-C L}^{-1}$  and  $\times 10^{-4} \text{ mol-C L}^{-1}$ ].

H. Name:  $a_{440}$ ,  $a_{350}$ ,  $a_{254}$

Description: The absorption coefficients at wavelengths 440 nm, 350 nm, and 254 nm, respectively. Absorbance (a) is a ratio measurement over a specific distance, where  $a = \log_{10}(I_0/I)/l$ , where  $I_0$  is the incident light intensity and  $I$  is the intensity of light after passing through the sample over the specified distance, 1 cm [units =  $\text{m}^{-1}$ ].

I. Name:  $\text{SUVA}_{254}$

Description:  $\text{SUVA}_{254}$  [units =  $\text{L mg C}^{-1} \text{ m}^{-1}$ ] is the specific ultraviolet (UV) absorbance at the wavelength 254 nm. It is computed as the ratio of the absorbance at 254 nm of the water sample [ $\text{m}^{-1}$ ] to the dissolved organic concentration [units =  $\text{mg-C L}^{-1}$ ].  $\text{SUVA}_{254}$  is reported in decadic [log-10] units.

J. Name: E2/E3

Description: E2/E3 [unitless] is the ratio of the light absorbance of the water sample at a wavelength of 250 nm to the absorbance at 365 nm measured by spectrophotometry.

K. Name: Fluorescence Index (FI)

Description: FI was calculated as the ratio of emission intensities at wavelengths 470 nm and 520 nm at an excitation of wavelength of 370 nm [unitless]. The wavelength of maximum emissions intensity is also given.

L. Name: Humification Index (HIX)

Description: HIX values were calculated using the following equation:

$$\text{HIX} = \frac{\int_{\text{em}=435\text{nm}}^{480\text{nm}} I_{\text{ex}=254\text{nm}}}{\int_{\text{em}=435\text{nm}}^{480\text{nm}} I_{\text{ex}=254\text{nm}} + \int_{\text{em}=300}^{345} I_{\text{ex}=254\text{nm}}}$$

Where  $I_{\text{ex}=254\text{nm}}$  represents the emission intensities at an excitation wavelength of 254 nm. HIX quantifies the degree to which emission red-shifts as humification (degradation from biological origin, shifting from low molecular weight bio-labile organics to more condensed aromatics through microbial action) occurs [unitless].

M. Name: Freshness Index ( $\beta/\alpha$ )

Description:  $\beta/\alpha$  was calculated as the ratio of emission intensities at 380 nm (marine- or algal-like, termed  $\beta$  or M components) to the maximum emission intensity between 420 – 435 nm (humic-like DOM, termed  $\alpha$  or C components) at an excitation wavelength of 310 nm [unitless].

N. Name: Ratio of peak C to peak A (C/A)

Description: C/A was calculated as the ratio of emission intensities at peak C (maximum emission intensity within excitation wavelengths = 300 – 360 nm and emission wavelengths = 420 – 460 nm) to peak A (maximum emission intensity within excitation wavelengths = 240 – 260 nm and emission wavelengths = 380 – 460 nm).

O. Name:  $R_a$

Description:  $R_a$  is the estimated rate of light absorption [units = mol-photons  $\text{L}^{-1} \text{s}^{-1}$ ] by the water samples in the solar simulator used throughout this study.  $R_a$  was estimated by chemical actinometry.

P. Name: [TMP]<sub>0</sub>

Description: The initial concentration of 2,4,6-trimethylphenol used to estimate the rate of triplet formation in all collected stormflow samples ( $\mu\text{M}$ )

Q. Name:  $k_{\text{obs,TMP}}$

Description:  $k_{\text{obs,TMP}}$  is the pseudo-first order rate constant for the photo-sensitized loss of 2,4,6-trimethylphenol (TMP) [units =  $\text{s}^{-1}$ ].

R. Name:  $\text{IF}_{\text{TMP}}$

Description: The estimated inhibition factor for the inhibition of  $^3\text{CDOM}^*$ -sensitized photolysis by DOC. All measurements that have been corrected for this inhibition have the superscript, c [unitless].

S. Name:  $k_{\text{obs,TMP}}^c$

- Description: The pseudo-first order rate constant for the photo-sensitized loss of 2,4,6-trimethylphenol (TMP) corrected for the inhibition of TMP photo-oxidation by DOC. Where  $k_{obs,TMP^c} = k_{obs,TMP}/IF_{TMP}$  [units =  $s^{-1}$ ].
- T. Name:  $R_{I,TMP^c}$   
 Description: The initial rate of loss of TMP where  $R_{I,TMP^c} = k_{obs,TMP^c} \times [TMP]_0$  [units =  $M s^{-1}$ ].
- U. Name:  $k_{T,TMP^c} \times [TMP]_0$   
 Description: The product of the second order rate constant,  $k_{T,TMP^c}$ , and the initial concentration of TMP,  $[TMP]_0$  [units =  $s^{-1}$ ].
- V. Name:  $k_q' + k_{T,TMP^c} \times [TMP]_0$   
 Description: The sum of the pseudo-first order rate constant for  ${}^3CDOM^*$  quenching,  $k_q'$ , and the reaction rate between  ${}^3CDOM^*$  and TMP,  $k_{T,TMP^c} \times [TMP]_0$ . This term describes the quenching/scavenging of  ${}^3CDOM^*$  with TMP present [units =  $s^{-1}$ ].
- W. Name:  $R_{f,T}$   
 Description: The rate of formation of triplet excited states of dissolved natural organic matter as measured by the photosensitized degradation of TMP [units =  $M s^{-1}$ ].
- X. Name:  $[{}^3CDOM^*]_{ss}$   
 Description:  $[{}^3CDOM^*]_{ss}$  is the steady-state concentration of triplet excited states of dissolved natural organic matter as determined from the photosensitized loss of TMP in the water samples under simulated sunlight [units =  $M$ ].
- Y. Name:  $AQY_T$   
 Description: The apparent quantum yield for the formation of triplet excited states of dissolved natural organic matter computed as the ratio of the rate of triplet formation to  $R_a$  [units =  $mol\ mol^{-1}\ photons^{-1}$ ].
- Z. Name:  $f_{TMP}$   
 Description:  $f_{TMP}$  is the quantum yield coefficient for TMP loss computed as the ratio of  $k_{obs,TMP}$  to  $R_a$  [units =  $L\ mol^{-1}\ photons^{-1}$ ]. In this samples set, it is used as a proxy for the efficiency of formation of triplet excited states of dissolved natural organic matter.
2. Worksheet: Spatial Variables
- A. Name: Longitude  
 Description: Longitudinal coordinates using World Geodetic System 1984 (WGS1984) datum.
- B. Name: Latitude  
 Description: latitudinal coordinates using World Geodetic System 1984 (WGS1984) datum.
- C. Name: Elevation  
 Description: Wetland elevation from digital elevation model (DEM) maps.
- D. Name: Terrestrial Ecosystem Classification  
 Description: Ecosystem classifications include: Northern Tallgrass Prairie (NTG), North Central Interior Oak Savannah (NCIOS), North Central Interior Maple Basswood Forest (NCIMBF), Central Mixedgrass Prairie (CMGP), Laurentian-

- Acadian Northern Harwood Forest (LANHF), Laurentian Pine-Oak Barren (LPOB), BWSFW=Boreal White Spruce Forest and Woodland (BWSFW). See reference: Sayre, R., P. Comer, H. Warner, and J. Cress (2009), A new map of standardized terrestrial ecosystems of the conterminous United States: U.S. Geological Survey Professional Paper 1768.
- E. Name: Cowardin System  
Description: A designation that, in general, describes the relative sizes of the freshwater wetlands. System designations include: Lacustrine (L) and Palustrine (P). See reference:  
Cowardin, L. M., V. Carter, F. C. Golet, and E. T. LaRoe. 1979. Classification of wetlands and deepwater habitats of the United States, United States Fish and Wildlife Service.
- F. Name: Cowardin Class  
Description: A general description of the vegetation. System designations include: forested (FO), scrub-shrub (SS), emergent (EM), aquatic bed (AB), unconsolidated bottom (UB).
- G. Name: Cowardin Water Regime (Hydroperiod)  
Description: A general description of the hydroperiods of the wetlands. Designations include: seasonally saturated (B), seasonally flooded (C), semi-permanently flooded (F), intermittently exposed (G), permanently flooded (H).
- H. Name: Hydrogeomorphic Class  
Description: A general designation of the landscape location of the wetlands. Terrene=headwater or hydrologically isolated wetland, Lentic=wetland within a lake basin, Lotic=wetland within an active floodplain. See reference:  
Tiner, R. W (2014), Dichotomous Keys and Mapping Codes for Wetland Landscape Position, Landform, Water Flow Path, and Waterbody Type Descriptors: Version 3.0. U.S. Fish and Wildlife Service, National Wetlands Inventory Program.
- I. Name: Hydrologic Connectivity  
Description: A designation of the surficial hydrologic connectivity. Throughflow: wetland has surface water inflow and outflow, Outflow: wetland has a surface water outflow (i.e., the wetland is a source of water to a stream), Vertical: wetland lacks surface water inflow or outflow.
- J. Name: Human Disturbance Score (HDS)  
Description: HDS is a qualitative measure of land use and wetland perturbations that accounts for the cumulative anthropogenic impacts on a wetland system. HDSs are empirically derived for individual sites using four ratings (best, moderate, fair, and poor) for five factors: (1) buffer landscape disturbance, (2) immediate landscape influence, (3) physical habitat alteration within the immediate landscape, (4) hydrological alteration, and (5) general chemical pollution factors. The HDS ranges between 0 (low or no human influence) to 100 (substantial human influence) and allows comparison of relative anthropogenic influences between wetland systems.
- K. Name: Watershed Area

- Description: Total area of the watershed draining to the delineated wetland area [units = km<sup>2</sup>].
- L. Name: Relative Impervious Cover (Impervious)  
Description: Relative area of impervious cover, such as roads, parking lots, and rooftops within a watershed [units = fraction].
- M. Name: Relative Wetland land cover (Wetland)  
Description: Relative area of palustrine wetlands with scrub-shrub, forested, and emergent vegetation within a watershed [units = fraction].
- N. Name: Relative Open Water land cover (Open Water)  
Description: Relative area of lakes, ponds, and rivers within a watershed [units = fraction].
- O. Name: Relative Forest land cover (Forest)  
Description: Relative area of coniferous, deciduous, and mixed forests within a watershed [units = fraction].
- P. Name: Relative Grassland land cover (Grassland)  
Description: Relative are of natural grassland, hay fields, pastureland, and manage grassland (parks and golf courses) within a watershed [units = fraction].
- Q. Name: Relative Cropland land cover (Cropland)  
Description: Relative are of row crop agriculture, such as corn, soybean, and wheat, within a watershed [units = fraction].
- R. Name: Slope  
Description: Average slope of a watershed reported as rise divided by run [units = %].
- S. Name: L/G  
Description: Average water flow path divided by the average slope. L/G is used as a proxy for the average watershed residence time of a watershed [units = km].
- T. Name: Soil organic matter  
Description: [units = %].
- U. Name: Clay  
Description: Weighted-average percent clay in the top 50-cm of soil in the watershed [units = %].
- V. Name: Sand  
Description: Weighted-average percent sand in the top 50-cm of soil in the watershed [units = %]
- W. Name: Silt  
Description: Weighted-average percent silt in the top 50-cm of soil in the watershed [units = %]
- X. Name: Net Primary Productivity  
Description: Ten-year average (2004 – 2014) average net primary productivity rates over the watershed area [units = kg-C m<sup>-2</sup> y<sup>-1</sup>]
3. Worksheet: Climate Variables
- A. Name: Site ID  
Description: Site identification name.

- B. Name: Month, Year, and Season  
Description: The month, year, and season in which a sample was collected.
- Y. Name: Longitude  
Description: Longitudinal coordinates using World Geodetic System 1984 (WGS1984) datum.
- Z. Name: Latitude  
Description: latitudinal coordinates using World Geodetic System 1984 (WGS1984) datum.
- C. Name: Mean Annual Temperature (MAT)  
Description: The average yearly temperature using the entire period of record at the nearest weather station (< 50 km) to each site [units = °C]. Data was accessed on the National Oceanic and Atmospheric Administration National Centers for Environmental Information webpage.
- D. Name: Mean Specific Year Temperature (MSYT)  
Description: The average temperature for the specific year in which a sample was collected [units = °C].
- E. Name: Mean Specific Month Temperature (MSMT)  
Description: The long-term average temperature for the specific month in which a sample was collected using the entire period of record [units = °C].
- F. Name: Specific Month Temperature (SMT)  
Description: The mean temperature for the specific month and year in which a sample was collected [units = °C].
- G. Name: Mean Annual Precipitation (MAP)  
Description: The average yearly precipitation using the entire period of record from a gridded database maintained by the Minnesota Department of Natural Resources [units = cm].
- H. Name: Mean Specific Year Precipitation (MSYP)  
Description: Average precipitation for the specific year in which a sample was collected [units = cm].
- I. Name: Mean Specific Month Precipitation (MSMP)  
Description: Long-term average monthly precipitation for the specific month in which a sample was collected using the entire period of record [units = cm].
- J. Name: Specific Month Precipitation (SMP)  
Description: The mean precipitation for the specific month and year in which a sample was collected [units = cm].