# EDI Metadata Template (2019)[[1]](#footnote-1)

Data should be in csv text file. If starting with an Excel spreadsheet, please make sure it does not contain any formulas and comments on cells. If you need comments put them in their own column. If data were used in a database and major table linking is necessary to analyze, please de-normalize into a flat file, not just database table exports.

## Dataset Title

(be descriptive, more than 5 words):

Time series of environmental parameters and organic matter analyses for dissolved and particulate organic matter in the Neuse River Estuary, North Carolina, USA 2015-2016

## Short name or nickname you use to refer to this dataset:

NRE stats dataset

## Abstract

(include what, why, where, when, and how)

Environmental parameters and organic matter analyses (concentration, absorbance, fluorescence) for dissolved and particulate organic matter for the Neuse River Estuary (North Carolina, USA) from 20 July 2015-28 July 2016. Samples were collected bi-weekly from July 2015-October 2015 and March 2016-July 2016 and monthly from November 2015-February 2016. The dataset consists of environmental parameters measured (water temperature, salinity, percent dissolved oxygen, turbidity, chlorophyll-a) and calculated (flushing time) as well as organic matter analyses for dissolved and particulate organic matter (concentration, absorbance, fluorescence) from surface (0.2 m below surface) and bottom (0.5 m above bottom) at 11 stations from the furthest extent of saltwater intrusion (Station 0) to the mouth of the estuary (Station 180). Data were collected as part of the Neuse River Estuary Modeling and Monitoring Program (ModMon; <http://paerllab.web.unc.edu/projects/modmon/>) at the University of Chapel Hill, Institute of Marine Science.

## Investigators

(list in order as for a paper with e-mail addresses, organization and preferably ORCID ID, if you don’t have one, get it, it’s easy and free: <http://orcid.org/>) add table rows as needed

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| First Name | Middle Initial | Last Name | Organization | e-mail address | ORCID ID (optional) |
| Alexandria | G. | Hounshell | Virginia Tech | alexgh@vt.edu | 0000-0003-1616-9399 |
| Hans | W. | Paerl | University of North Carolina – Chapel Hill | hans\_paerl@unc.edu | 0000-0003-2211-1011 |
| Nathan | S. | Hall | University of North Carolina – Chapel Hill | nshall@unc.edu |  |
| Jeremey | S. | Braddy | University of North Carolina – Chapel Hill | jbraddy@email.unc.edu |  |
| Karen | L. | Rossignol | University of North Carolina – Chapel Hill | krossign@email.unc.edu |  |
| Randy |  | Sloup | University of North Carolina – Chapel Hill | randys@email.unc.edu |  |

## Other personnel names and roles

(dataset creators & contact, field crew, data entry etc. with e-mail addresses, organization and ORCID ID)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| First Name | Middle Initial | Last Name | Organization | e-mail address | ORCID ID (optional) | Role in project |
| N/A |  |  |  |  |  |  |
|  |  |  |  |  |  |  |

## License

(Select a license for release of your data. We have 2 recommendations: [CCO – most accommodating of data reuse](https://creativecommons.org/publicdomain/zero/1.0/), & [CCBY – requires attribution](https://creativecommons.org/licenses/by/4.0/))

CCBY

## Keywords

(List keywords and separate with commas. Using keywords from a controlled vocabulary (CV) will improve the future discovery and reuse of your data. The LTER CV is effective at describing ecological and environmental data. [Access the LTER CV here](http://vocab.lternet.edu/vocab/vocab/index.php). [Try this text mining service to extract LTER CV keywords from your abstract or methods](http://vocab.lternet.edu/keywordDistiller/). Additionally, please determine one or two keywords that best describe your lab, station, and/or project (e.g., Trout Lake Station, NTL LTER). This will help others discover your data by site/project).

University of North Carolina – Chapel Hill, ModMon, Neuse River Estuary, salinity, turbidity, water temperature, dissolved oxygen, chlorophyll-a, dissolved organic matter, particulate organic matter, absorbance, fluorescence

## Funding of this work:

Add rows to table if several grants were involved, list only the main PI, start with main grant first:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| PI First Name | PI Middle Initial | PI Last Name | PI ORCID ID (optional) | Title of Grant | Funding Agency | Funding Identification Number |
| Alexandria | G | Hounshell | 0000-0003-1616-9399 | USGS-WRRI Fellowship | North Carolina Water Resources Research Institute |  |
| Hans | W | Paerl | 0000-0003-2211-1011 |  | North Carolina Sea Grant Program | Project R/MG-1505 |
| Hans | W | Paerl | 0000-0003-2211-1011 |  | North Carolina Dept. of Environmental Quality/National Fish and Wildlife Foundation | 8020.16.053916 |
| Hans | W | Paerl | 0000-0003-2211-1011 | Neuse River Estuary Monitoring and Modeling Project |  |  |
| Hans | W | Paerl | 0000-0003-2211-1011 | NSF RAPID | National Science Foundation, Division of Ocean Sciences | OCE-1705972 |

## Timeframe

* Begin date: 20 July 2015
* End date: 28 July 2016
* Data collection ongoing/completed: Completed

## Geographic location

* Verbal description: Neuse River Estuary, North Carolina, USA
* North bounding coordinates (decimals): 35.223531
* South bounding coordinates (decimals): 34.914575
* East bounding coordinates (decimals): -77.153169
* West bounding coordinates (decimals): -76.485125

## Taxonomic species or groups

N/A

## Methods

(please be specific, include instrument descriptions, or point to a protocol online, if this is a data compilation please specify datasets used, preferably their DOI or URL plus general citation information)

Samples for physical, chemical, biological, and organic matter (dissolved and particulate organic matter, DOM and POM respectively) analyses were collected as part of the Neuse River Monitoring and Modeling Program (ModMon; http://paerllab.web.unc.edu/projects/modmon/) conducted by the University of North Carolina – Chapel Hill, Institute of Marine Sciences (UNC-CH IMS) (Paerl et al. 2018). Samples were collected from July 20, 2015 to July 28, 2016; bi-weekly from March through October and monthly from November through February. For each sampling date (n = 22), samples were collected at 11 stations in the NRE spanning the upstream-most location of salinity intrusion (Station 0) to the mouth of the estuary (Station 180). In situ measurements (water temperature, salinity, turbidity, percent dissolved oxygen) were collected at discrete depths on the sunlit side of the research vessel using a Yellow Springs Instruments (YSI Incorporated, Ohio) multiparameter sonde (Model 6600 or 6600 EDS-S Extended Deployment System) equipped with a YSI conductivity/temperature probe (Model 6560), a YSI pulsed dissolved oxygen probe (Model 6562), and a self cleaning YSI turbidity probe (Model 6026 or 6136). The YSI sonde was coupled to a either a YSI 610 DM datalogger or a YSI 650 MDS Multi-parameter Display System datalogger. In situ measurements were performed at the surface (approximately 0.2 meters) and at the bottom of the water column (approximately 0.5 meters from the sediment layer).

For each sampling date, a surface (0.2 m below surface) and bottom (0.5 m above bottom) water sample were collected for chemical, biological, and organic matter analyses at each of the 11 stations using a peristaltic pump. Samples were maintained in the dark at ambient temperature and returned to UNC-CH Institute of Marine Sciences within ~6 hours of collection. Samples were filtered through pre-combusted (450 degrees C, 4 h) GF/F glass fiber filters (0.7 µm nominal pore size). The filtrate was collected and stored frozen at -20°C in the dark until dissolved nutrient and DOM quantitative and qualitative analysis. Filters were collected and stored frozen at -20 degrees C in the dark until chlorophyll-a analysis, conducted within one month of collection, and POM quantitative and qualitative analysis, as described below.

The freshwater flushing time for each station and date was calculated using the date-specific fraction of freshwater method (Alber and Sheldon, 1999) as described in Peierls et al. 2012. Briefly, the date-specific average discharge is an iterative calculation that averages the riverine discharge over the flushing time period.

Organic matter analysis

DOC concentration ([DOC]) was measured via high-temperature catalytic oxidation on a Shimadzu TOC-5000 analyzer (Peierls et al. 2003): Water samples were vacuum filtered (less than 25 kilopascal) using pre-combusted Whatman glass microfiber filters (GF/F). The filtrate was stored in pre-combusted glass scintillation vials with Teflon closures and frozen at -20 degrees Celsius until analysis. The Shimadzu TOC-5000A Analyzer uses high temperature catalytic oxidation followed by non-dispersive infrared analysis of the CO2 produced. Samples were acidified to a pH less than 2 and sparged with air before they were analyzed for non-volatile organic carbon. Total dissolved nitrogen (TDN), nitrate + nitrite, and ammonium were determined colorimetrically using a Lachat QuickChem autoanalyzer (Peierls et al. 2003). Dissolved organic nitrogen ([DON]) was determined by subtracting the dissolved inorganic nitrogen species (DIN, as nitrate + nitrite and ammoinium) from TDN. The molar ratio of dissolved organic carbon (DOC) to dissolved organic nitrogen (DON) or DOC:DON was calculated.

Particulate organic carbon concentration ([POC]) and particulate nitrogen ([PN]) were determined on one set of collected filters via high temperature combustion on a Costech ECS 4010 analyzer, after vapor acidification (HCl) to remove carbonates (Paerl et al., 2018). After drying at 60 degrees C, the filters were rolled in tin disks and injected into a Costech Analytical Technologies, Inc. Elemental Combustion System CHNS-O ECS 4010 for elemental analysis. Atropine standards were used to develop a calibration curve (C 70.56%, N 4.84%, and carbon response ratio of 0.025 +/-0.003). NIST Buffalo River Sediment Reference Material 8704 (C 3.351% +/-0.017, N 0.20% +/-0.04) and/or Acetanilide Bypass (C 71.09%, N 10.36%, carbon response ratio of 0.055 +/- 0.003) were used for calibration or as a check standard.

Samples for fluorescent base-extracted particulate organic matter (BEPOM) were extracted following Osburn et al. 2012. Briefly, seston on collected filters was extracted using 10 mL of 0.1 M NaOH and stored in the dark at 4 degrees C for 24 hours. Samples were then neutralized with concentrated HCl (~ 100 µL) to measured neutral pH (~ 7.0) and filtered through 0.2 µm porosity, PES filters. Filtered extracts were immediately analyzed for absorbance and fluorescence as described below. For absorbance and fluorescence, DOM and neutralized BEPOM samples were filtered through 0.2 µm mesh size, polyethersulfone (PES) filters immediately prior to analysis to ensure optical consistency.

Absorbance spectra for filtered DOM and extracted BEPOM samples were measured on a Shimadzu UV-1700 Pharma-Spec spectrophotometer. Absorbance spectra were corrected using a Nanopure water blank measured at the beginning of each day of analysis. All samples with > 0.4 raw absorbance units at 240 nm were diluted, and final results were corrected for dilution (Osburn et al. 2012). Absorbance values at 254 nm were converted to Napierian absorbance coefficients (aλ, 1/m) (Spencer et al. 2013). Specific UV absorbance (SUVA254) (L/mg C/m) was calculated as decadal a254/[OC] (as [DOC] or [POC], respectively) for each sample (Weishaar et al. 2003).

Fluorescence spectra (i.e., excitation-emission matrices, EEMs) were measured on a Varian Cary Eclipse spectrofluorometer. Excitation wavelengths were scanned from 240 to 450 nm at 5 nm increments, and emission wavelengths were scanned from 300 to 600 nm at 2 nm increments. Instrument excitation and emission corrections were applied to each sample in addition to corrections for inner-filtering effects, calibrated against the Raman signal of Nanopure water, and standardized to quinine sulfate equivalents (Q.S.E.) (Murphy et al. 2013).

The humification index (HIX) and biological index (BIX) were calculated from measured fluorescence spectra and used as indicators of the relative quality of OM in estuaries from more terrestrial, humic-like OM to more biological, autochthonously produced OM (Huguet et al. 2009). HIX is the ratio of the H (435-480 nm) and L (300-345 nm) regions of fluorescence measured at an excitation wavelength of 254 nm. HIX is indicative of the degree of humification and aromaticity of the fluorescent organic matter (OM) in a sample and generally decreases down estuary. BIX is calculated as the ratio between the β (380 nm) (Peak M) and α (430 nm) (Peak C) regions of fluorescence measured at an excitation wavelength of 310 nm. BIX is an indicator of autochthonous, recently produced fluorescent OM and generally increases down estuaries (Huguet et al. 2009). In addition to fluorescent indicators such as HIX and BIX, peak-picking methods were used to identify previously selected and characterized EEM fluorescent peaks from the literature (Coble 2007; Fellman et al. 2010) via in-house Matlab scripts.

Chlorophyll-a (Chl a) analysis

Chl a concentration was measured using the modified in vitro fluorescence technique in EPA Method 445.0 (Welshmeyer 1994, Arar et al. 1997): Fifty milliliters of each water sample were vacuum filtered (less than 25 kilopascals) through duplicate filters at low ambient light conditions using 25 mm Whatman glass microfibre filters (GF/F). The filters were blotted dry, wrapped in foil and frozen immediately at -20 degrees C until analysis. Chl a was extracted from the filter using a tissue grinder and 10 mL of 90 percent reagent grade aqueous acetone. The samples remained in the acetone overnight at -20 degrees C. The extracts were filter-clarified using a centrifuge and analyzed on a Turner Designs TD-700 fluorometer that was configured for the non-acidification method of Welschmeyer (1994). The value reported is the average Chl a concentration measured from the two filters. The fluorometer was calibrated with a known concentration of pure Chl a that was determined using a TurnerDesigns Trilogy fluorometer. The calibration was checked daily against a solid secondary standard.

References

Alber, M., Sheldon, J.E., 1999. Use of a date-specific method to examine variability in the

flushing times of Georgia estuaries. Estuarine, Coastal and Shelf Science. 49, 469–482.

Arar, E.J., Collins, G.B., 1997. In Vitro Determination of Chlorophyll a and Pheophytin a in Marine and Freshwater Algae by Fluorescence. EPA Method 445.0. Technical report for USA-EPA, Cincinnati, Ohio, September 1997.

Coble, P.G., 2007. Marine optical biogeochemistry: The chemistry of ocean color. Chemical Reviews 107, 402–418. <https://doi.org/10.1021/cr050350>

Fellman, J.B., Hood, E., Spencer, R.G.M., 2010. Fluorescence spectroscopy opens new windows into dissolved organic matter dynamics in freshwater ecosystems: A review. Limnology and Oceanography 55, 2452–2462. <https://doi.org/10.4319/lo.2010.55.6.2452>

Huguet, A., Vacher, L., Relexans, S., Saubusse, S., Froidefond, J.M., Parlanti, E., 2009. Properties of fluorescent dissolved organic matter in the Gironde Estuary. Organic Geochemistry 40, 706–719. <https://doi.org/10.1016/j.orggeochem.2009.03.002>

Murphy, K.R., Stedmon, C.A., Graeber, D., Bro, R., 2013. Decomposition routines for Excitation Emission Matrices. Analytical Methods 5(23), 1–29. <https://doi.org/10.1039/c3ay41160e.drEEM>

Osburn, C.L., Handsel, L.T., Mikan, M.P., Paerl, H.W., Montgomery, M.T., 2012. Fluorescence tracking of dissolved and particulate organic matter quality in a river-dominated estuary. Environmental Science & Technology 46, 8628–8636. https://doi.org/10.1021/es3007723

Paerl, H.W., Crosswell, J.R., Dam, B. Van, Hall, N.S., Rossignol, K.L., Osburn, C.L., Hounshell, A.G., Sloup, R.S., Harding, L.W., 2018. Two decades of tropical cyclone impacts on North Carolina’s estuarine carbon, nutrient and phytoplankton dynamics: implications for biogeochemical cycling and water quality in a stormier world. Biogeochemistry 141(3), 307-332. <https://doi.org/10.1007/s10533-018-0438-x>

Peierls, B.L., Christian, R.R., Paerl, H.W., 2003. Water Quality and Phytoplankton as Indicators of Hurricane Impacts on a Large Estuarine Ecosystem. Estuaries 26, 1329–1343. https://doi.org/10.1007/BF02803635

Peierls, B.L., Hall, N.S., Paerl, H.W., 2012. Non-monotonic Responses of Phytoplankton Biomass Accumulation to Hydrologic Variability: A Comparison of Two Coastal Plain North Carolina Estuaries. Estuaries and Coasts 1–17. <https://doi.org/10.1007/s12237-012-9547-2>

Spencer, R.G.M., Aiken, G.R., Dornblaser, M.M., Butler, K.D., Holmes, R.M., Fiske, G., Mann, P.J., Stubbins, A., 2013. Chromophoric dissolved organic matter export from U.S. rivers. Geophysical Research Letters 40, 1575–1579. <https://doi.org/10.1002/grl.50357>

Weishaar, J.L., Fram, M.S., Fujii, R., Mopper, K., 2003. Evaluation of Specific Ultraviolet Absorbance as an Indicator of the Chemical Composition and Reactivity of Dissolved Organic Carbon. Environmental Science & Technology 4702–4708. https://doi.org/10.1021/es030360x

Welschmeyer, N.A. 1994. Fluorometric analysis of chlorophyll a in the presence of chlorophyll b and pheopigments. Limnology and Oceanography 39, 1985-1992.

## Data Table

* Column name: exactly as it appears in the dataset. Please avoid special characters, dashes and spaces.
* Description: please be specific, it can be lengthy
* Unit: please avoid special characters and describe units in this pattern: e.g. microSiemenPerCentimeter, microgramsPerLiter, absoptionPerMolePerCentimeter
* Code explanation: if you use codes in your column, please explain in this way: e.g. LR=Little Rock Lake, A=Sample suspect, J=Nonstandard routine followed
* Data format: please tell us exactly how the date and time is formatted: e.g. mm/dd/yyyy hh:mm:ss plus the time zone and whether or not daylight savings was observed.
* If a code for ‘no data’ is used, please specify: e.g. -99999

Please add rows as needed

**Table description:** Add a description for each table

NRE Multistats

|  |  |  |  |
| --- | --- | --- | --- |
| Column name | Description | Unit or  code explanation or date format | Empty value code |
| Date | Date of water sample collection, filtration, and in situ measurements.  Water sampling was conducted bi-weekly (March-October) and monthly (November-February). | mm/dd/YYYY | NA |
| Season | The season when the water sample was collected and filtered and when the *in situ* measurements were performed in the field. | Winter = December-February  Spring = March-May  Summer = June-August  Fall = September-November | NA |
| Station | The name of the fixed sampling station. | Station names decrease in number (in increments of 10) from 180 (the most downstream station sampled) to 0 (the most upstream station sampled). | NA |
| Depth | Depth from which the water sample was collected and where the in situ measurements were made. | S = surface (0.2 m below surface)  B = bottom (0.5 m above sediment layer) | NA |
| DepthNum | Depth converted to a number for data analysis. | 1 = Surface  2 = Bottom | NA |
| Temp\_C | In situ water temperature | degreesCelsius | NA |
| Sal\_ppt | In situ salinity | partsPerThousand | NA |
| DO\_mgL | In situ dissolved oxygen concentration | milligramsPerLiter | NA |
| DO\_Sat | In situ percent saturation dissolved oxygen | percentSaturation | NA |
| Turb\_NTU | In situ turbidity | nephlometricTurbidityUnits | NA |
| Chla\_ugL | Chlorophyll *a* concentration measured by in vitro fluorometry | microgramsPerLiter | NA |
| FlushingTime\_d | Freshwater flushing time | day | NA |
| DOC\_uM | Dissolved organic carbon concentration | microMolar | NA |
| DOC\_mgL | Dissolved organic carbon concentration | milligramsPerLiter | NA |
| DON\_ugL | Dissolved organic nitrogen concentration | microgramsPerLiter | NA |
| DON\_mgL | Dissolved organic nitrogen concentration | milligramsPerLiter | NA |
| DOCtoDON | Molar ratio of dissolved organic carbon to dissolved organic nitrogen | Unitless | NA |
| a254\_DOM | Naperian absorbance coefficients at 254 nm for DOM | perMeter | NA |
| SUVA\_DOM | SUVA for DOM | litersPerMilligramCarbonPerMeter | NA |
| HIX\_DOM | Humification index for DOM | Unitless | NA |
| BIX\_DOM | Biological index for DOM | Unitless | NA |
| Max\_FL\_DOM | Maximum fluorescent intensity for each excitation emission matrix for DOM | quinineSulfateUnits | NA |
| B\_DOM | Fluorescent intensity measured at Ex = 275 nm; Em = 310 nm for DOM | quinineSulfateUnits | NA |
| T\_DOM | Fluorescent intensity measured at Ex = 275 nm; Em = 340 nm for DOM | quinineSulfateUnits | NA |
| A\_DOM | Fluorescent intensity measured at Ex = 260 nm; Em = 380-460 nm for DOM | quinineSulfateUnits | NA |
| C\_DOM | Fluorescent intensity measured at Ex = 320-360 nm; Em = 370-410 nm for DOM | quinineSulfateUnits | NA |
| M\_DOM | Fluorescent intensity measured at Ex = 290-310 nm; Em = 370-410 nm for DOM | quinineSulfateUnits | NA |
| N\_DOM | Fluorescent intensity measured at Ex = 280 nm; Em = 370 nm for DOM | quinineSulfateUnits | NA |
| POC\_uM | Particulate organic carbon concentration | microgramsPerLiter | NA |
| POC\_mgL | Particulate organic carbon concentration | milligramsPerLiter | NA |
| PN\_uM | Particulate nitrogen concentration | microgramsPerLiter | NA |
| PN\_mgL | Particulate nitrogen concentration | milligramsPerLiter | NA |
| POCtoPN | Molar ratio of particulate organic carbon to particulate nitrogen | Unitless | NA |
| a254\_POM | Naperian absorbance coefficients at 254 nm for POM | perMeter | NA |
| SUVA\_POM | SUVA for POM | litersPerMilligramCarbonPerMeter | NA |
| HIX\_POM | Humification index for POM | Unitless | NA |
| BIX\_POM | Biological index for POM | Unitless | NA |
| Max\_FL\_POM | Maximum fluorescent intensity for each excitation emission matrix for POM | quinineSulfateUnits | NA |
| B\_POM | Fluorescent intensity measured at Ex = 275 nm; Em = 310 nm for POM | quinineSulfateUnits | NA |
| T\_POM | Fluorescent intensity measured at Ex = 275 nm; Em = 340 nm for POM | quinineSulfateUnits | NA |
| A\_POM | Fluorescent intensity measured at Ex = 260 nm; Em = 380-460 nm for POM | quinineSulfateUnits | NA |
| C\_POM | Fluorescent intensity measured at Ex = 320-360 nm; Em = 370-410 nm for POM | quinineSulfateUnits | NA |
| M\_POM | Fluorescent intensity measured at Ex = 290-310 nm; Em = 370-410 nm for POM | quinineSulfateUnits | NA |
| N\_POM | Fluorescent intensity measured at Ex = 280 nm; Em = 370 nm for POM | quinineSulfateUnits | NA |

## Articles

(List articles citing this dataset)

|  |  |  |
| --- | --- | --- |
| Article DOI or URL (DOI is preferred) | Article title | Journal title |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  |  |

## Scripts/code (software)

(List any software scripts/code you would like to archive along with your data. These may include processing scripts you wrote to create, clean, or analyze the data.)

|  |  |  |
| --- | --- | --- |
| File name | Description | Scripting language |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  |  |

## Data provenance

(Were these data derived from other data? If so, you will want to document this information so users know where these data come from.)

|  |  |  |  |
| --- | --- | --- | --- |
| Dataset title | Dataset DOI or URL | Creator (name & email) | Contact (name & email) |
| N/A |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |

## Notes and Comments

1. This document liberally borrows from similar documents at SBC and GCE [↑](#footnote-ref-1)