#### **Title**

Spatial Study 2021: Sample-Based Surface Water Dissolved Inorganic Carbon, Dissolved Organic Carbon, Total Nitrogen, Total Suspended Solids, Ions, and Organic Matter Characterization from across Multiple Watersheds in the Yakima River Basin, Washington, USA (v2)

# Summary

This dataset supports a broader study examining the drivers of spatial variability in sediment respiration rates in the Yakima River Basin. The dataset provides geochemistry and organic matter characterization data generated from samples collected during the same two-week period at 47 sites within multiple rivers throughout the Yakima River Basin in Washington, USA. Related sensor data will be published separately and can be used to link sediment respiration rates to biogeochemical processing rates.

### **Data Package Structure**

This dataset is comprised of one main data folder containing (1) file-level metadata; (2) data dictionary; (3) field metadata; (4) dissolved inorganic carbon (DIC), dissolved organic carbon (DOC; reported as non-purgeable organic carbon; NPOC), total nitrogen (TN), total suspended solids (TSS), and ions; (5) averaged values from water chemistry data; (6) surface water sampling protocol; (7) sensor protocol (8) readme; (9) methods codes; (10) international geo-sample number (IGSN) mapping file; and (11) folder of high resolution characterization of organic matter via 12 Tesla Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS) through the Environmental Molecular Sciences Laboratory (EMSL; <a href="https://www.pnnl.gov/environmental-molecular-sciences-laboratory">https://www.pnnl.gov/environmental-molecular-sciences-laboratory</a>). This folder contains two subfolders, one containing the .xml data files and the other containing instructions for using Formularity (https://omics.pnl.gov/software/formularity) and an R script to process the data based on the user's specific needs. All files are .csv, .pdf, .R, .ref, or .xml.

## **Acknowledgements**

We acknowledge the Yakama Nation as owners and caretakers of the lands where we collected our data. We thank the Confederated Tribes and Bands of the Yakama Nation Tribal Council and Yakama Nation Fisheries for working with us to facilitate sample collection and optimization of data usage according to their values and worldview.

This research was supported by the U.S. Department of Energy (DOE) Biological and Environmental Research (BER) Environmental System Science (ESS) program (<a href="https://ess.science.energy.gov/">https://ess.science.energy.gov/</a>) through the Pacific Northwest National Laboratory River Corridor Science Focus Area (SFA). PNNL is operated by Battelle Memorial Institute for the U.S. Department of Energy under Contract No. DE-AC05-76RL01830. FTICR-MS data was generated at the DOE BER Environmental Molecular Science Laboratory User Facility under user proposal 60221.

#### **Contact**

James Stegen, james.stegen@pnnl.gov

# **Change History**

Version 2	September 2022	Original data package publication

Version 2	May 2023	•	Revised DIC, NPOC, and TN data and summary data files. Original data used QAQC approach (blank correction) that has been removed.
	146	•	Removed blank correction methods deviation from ion data and methods codes file. The ion data (original v1 and current v2) were not blank corrected.
		•	Updated title, readme, and flmd to reflect changes.