Title

Data and scripts associated with “Riverine dissolved organic matter transformations increase with watershed area, water residence time, and Damköhler numbers in nested watersheds”

Summary

This data package is associated with the publication “Riverine dissolved organic matter transformations increase with watershed area, water residence time, and Damköhler numbers in nested watersheds” submitted to Biogeochemistry by Ryan et al., 2024 (pre-print DOI: 10.22541/essoar.171164898.83027743/v1). Once the paper is published, the new DOI will be added to this abstract and to the citations feature.

This study aims to investigate fundamental and transferable drivers of dissolved organic matter (DOM) diversity across five nested watersheds within the contiguous United States. DOM diversity was explored using ultrahigh-resolution Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS). The samples and the unprocessed FTICR-MS data used in this study are publicly available on the Environmental System Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) data repository (see DOIs below). The data for the Willamette, Gunnison, Connecticut, and Deschutes basins were collected as part of a collaboration between the Watershed Rules of Life (WROL) project and Worldwide Hydrobiogeochemistry Observation Network for Dynamic River Systems (WHONDRS). The data for the Yakima River basin (YRB) was collected by the PNNL River Corridor SFA. The raw, unprocessed FTICR-MS data with additional (meta)data can be found at doi:10.15485/1895159 for WROL samples and doi:10.15485/1898912 for YRB samples. This data package contains the processed data used in the associated manuscript. This data package is associated with the GitHub repository found at https://github.com/WHONDRS-Hub/rcsfa-RC4-WROL-YRB_DOM_Diversity.

Brief Overview of Methods

For a full description of the methods, see the methods section in Ryan et al., 2024. Briefly, water samples were collected at 52 sites within five nested watersheds located in the contiguous United States. Samples were analyzed for dissolved organic carbon (DOC) and dissolved organic matter (DOM) chemistry via ultrahigh-resolution Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS). DOM data were used to infer putative biochemical transformations following methods previously published in Garayburu-Caruso et al., 2020. Patterns in DOM molecular diversity and putative biochemical transformations were assessed across gradients of explanatory variables associated with watershed characteristics (e.g., watershed area, water residence time, land cover) to investigate fundamental and transferable drivers of DOM diversity across watersheds.

Data Package Structure

At the directory level, the data package is comprised of three folders: (1) data, (2) output, and (3) src; and five additional files including the data dictionary (file ending in "_dd.csv”) and file-level metadata (file ending in “_flmd.csv”). The “src” folder contains the scripts used to process the FTICR data, conduct the analyses, and produce the manuscript figures. The inputs for these scripts are in the “data” folder and the returned outputs in the “output” folder. Inputs include temporal and spatial metadata associated with the sampling efforts, processed FTICR data, and total and normalized putative biochemical transformations per sample. Outputs include cleaned and combined data presented as tables, descriptive statistics, and plots. The file-level metadata file lists all files contained in this data

package and descriptions for each. The data dictionary describes the units and definitions for each tabular data column or row header .

Citations and Acknowledgements

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Cite this data package with the appropriate DOI. Cite the associated manuscript in any work that that uses analyses or conclusions presented in the manuscript. The pre-print manuscript citation is listed below. Once the published manuscript is available, you can find the updated citation on this data package's ESS-DIVE landing page.

Ryan, K. A., Garayburu-Caruso, V. A., Crump, B. C., Bambakidis, T., Raymond, P. A., Liu, S., & Stegen, J. C. (2024). Riverine dissolved organic matter transformations increase with watershed area, water residence time, and Damköhler numbers in nested watersheds. ESS Open Archive. Pre-print DOI: 10.22541/essoar.171164898.83027743/v1

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Otenburg O ; Barnes M ; Borton M A ; Chen X ; Chu R ; Farris Y ; Forbes B ; Fulton S G ; Garayburu-Caruso V A ; Goldman A E ; Gonzalez B I ; Grieger S ; Kaufman M H ; McKever S A ; Myers-Pigg A ; Pelly A ; Renteria L ; Scheibe T D ; Son K ; Torgeson J M ; Toyoda J G ; Stegen J C (2022): Temporal Study 2021-2022: Sample-Based Surface Water Chemistry and Organic Matter Characterization across Watersheds in the Yakima River Basin, Washington, USA (v2). River Corridor and Watershed Biogeochemistry SFA, ESS-DIVE repository. Dataset. doi:10.15485/1898912 accessed via https://data.ess-dive.lbl.gov/datasets/doi:10.15485/1898912

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Change History

Data Package Version	Changes
Version 1 *August 2024*	Original data package publication