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.

Critical Details

The following steps were followed to generate the processed FTICR-MS data:

1 – The raw, unprocessed FTICR-MS data (XML files) were downloaded for WROL (doi:10.15485/1895159) and YRB (doi:10.15485/1898912) samples from ESS-DIVE.

2 – The instructions in the "FTICR_Instructions-Report_Generation_SOP_v3.pdf" document found in the original data packages were followed. Molecular formulae were assigned using Formularity software.

The data were further processed, and sample molecular properties were assigned using the R package “ftmsRanalysis”.

- The outputs from these steps were put into a folder called "Formularity_Output_Folder". This folder is not found within this data package but is referenced in “Removing_poorly_calibrated_and_merge_reps.R" (see next step). If the user wants to create the processed data files with all replicates and before poorly calibrated samples were removed, they will need to follow these steps to create the processed data within a folder called "Formularity_Output_Folder".

3 – Poorly calibrated samples were removed from the dataset and sample replicates from each site were merged such that a peak was kept in the merged sample if it was present in at least one of the reps. This step is computed within the “Removing_poorly_calibrated_and_merge_reps.R” script.

4 – Putative biochemical transformations were inferred following protocols previously described in Garayburu-Caruso et al. (2020). Briefly, pairwise mass differences were calculated between every peak (with and without molecular formula assigned) in a merged sample and compared to a reference list of reference transformations (“Transformation_Database_07-2020.csv”). Mass differences were matched to the compounds in the reference list (within 1 ppm) to infer the gain or loss of that compound via a biochemical transformation.

5 – Total number of transformations per sample and total number of transformations normalized per number of peaks in a sample were calculated.

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, the updated citation can be found on this data package's landing page on ESS-DIVE.

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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Citations:

- Garayburu-Caruso, V.A.; Danczak, R.E.; Stegen, J.C.; Renteria, L.; Mccall, M.; Goldman, A.E.; Chu, R.K.; Toyoda, J.; Resch, C.T.; Torgeson, J.M.; et al. Using Community Science to Reveal the Global Chemogeography of River Metabolomes. *Metabolites* 2020, *10*, 518. https://doi.org/10.3390/metabo10120518
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Change History

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