

Title

FTICR-MS Data from Multi-continent River Water and Sediment and from Coastal River Fresh and Saline Sediment Associated with: "Dissolved Organic Matter Functional Trait Relationships are Conserved Across Rivers"

Summary

This data package is associated with the publication "Dissolved Organic Matter Functional Trait Relationships are Conserved Across Rivers" submitted to PNAS (Stegen et al., 2023). The study aims to understand large-scale spatial structure of the dissolved organic matter (DOM) thermodynamic traits and inter-trait relationships by investigating (1) river water and sediments collected along 97 rivers spanning 3 continents and (2) coastal sediment collected from fresh and saline locations in Pacific and Gulf/Atlantic rivers. Sediment extracts and water samples were analyzed using ultrahigh resolution Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS). This dataset is comprised of three folders (1) Coastal, (2) WHONDR_S19S, and (3) Data_Dictionaries. Coastal contains (1) a subfolder with processed FTICR-MS data as csv files and sample collection metadata, (2) a subfolder with R scripts used to process the data and create associated figures, (3) a subfolder with the raw, unprocessed FTICR-MS data as .xml files, and (4) a readme file with more information about the dataset and instructions for using Formularity (<https://omics.pnl.gov/software/formularity>). WHONDRS_S19S contains (1) a csv file with processed FTICR data, (2) a csv with sample collection metadata, (3) a csv with sample geospatial data, (4) a csv with simulated lambda model outputs, (5) a subfolder with R scripts used to process the data and create associated figures, and (6) a readme file with more information regarding WHONDRS raw FTICR data and processing scripts. Data_Dictionaries contains data dictionaries for each csv file in the data package. The 97 global river corridors were part of a WHONDRS (<https://whondrs.pnnl.gov>) study. The raw, unprocessed FTICR-MS data with additional data can be found at doi:10.15485/1729719 for sediments and doi:10.15485/1603775 for water. This data package contains the processed data used in the associated manuscript. The coastal data has not been previously published, and this data package contains both the raw and processed data.

Data Package Structure

Please see FLMD.csv for a list of all files contained in this data package and descriptions for each. Data dictionaries for csv files have "_dd" appended to the file names.

Citations and Acknowledgements

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Change History

Version 1	28 Sept 2021	Original data package publication
Version 2	14 Oct 2022	Changed the title of the data package. Added WHONDRS Geospatial data and data dictionary. Added scripts linked to new analysis
Version 3	02 Feb 2023	Changed the title of the data package. Added scrips and data linked to new analysis