Title

Data and scripts associated with: “Burn severity and vegetation type control phosphorus concentration, molecular composition, and mobilization”

Summary

This data package is associated with the publication “Burn severity and vegetation type control phosphorus concentration, molecular composition, and mobilization” published in European Geophysical Union - Biogeosciences (Barnes et al. 2025).

This study investigates how phosphorus (P) biogeochemistry is altered by burn severity in contrasting types of vegetation chars. This data package documents the workflow used to process and generate the main figures and statistics in the manuscript. The R scripts reference minimally processed P nuclear magnetic resonance (P-NMR) and X-ray absorption near edge structure (P-XANES) data, as well as fully processed data including total elemental composition of the solid chars, total elemental composition of the char leachates (particulate and aqueous phases), and leachate aqueous phase molybdate reactive P concentration. These source data and associated metadata can be found on ESS-DIVE at https://data.ess-dive.lbl.gov/datasets/doi:10.15485/1894135 (Grieger et al. 2022; v3). Files and scripts included in this data package finish the processing workflow for P-NMR and P-XANES data. These data can be used to gain a better understanding of bulk chemical changes in chars and their leachates, as well as detailed molecular changes to P.

This data package is associated with the GitHub repository found at https://github.com/river-corridors-sfa/rcsfa-RC3-BSLE_P.

Brief Overview of Methods

This study uses a subset of samples from Grieger et al. (2022); refer to Grieger et al. (2022) for details on the experimental design and the meaning behind the sample names Douglas-fir (*Pseudotsuga menziesii*) and sagebrush (*Artemisia tridentata*) vegetation was collected from the field and burned on open air tables under varying burning conditions to generate chars. Char burn severity was classified according to US Forest Service field metrics. Total elemental analysis (P, sulfur, aluminum, iron, magnesium, calcium, sodium, and potassium) of the solid chars was measured using an inductively coupled plasma optical emission spectrometer (ICP-OES). Solution-state ^{31}P NMR experiments were conducted on char extracts and P-XANES was collected on intact solid samples. Unburned vegetation and chars were leached with synthetic rainwater to simulate what might be mobilized from the solid material during rain events. Leachates were filtered through a coarse mesh followed by a nominal 0.7 micrometers (µm) pore size. Coarse filtered and < 0.7 µm filtered leachates were ran for total elemental analyses using ICP-OES. Total elemental concentration of the leachate particulate phase (2 mm to 0.7 µm) was calculated as the difference between the coarse filtered and aqueous phase. Molybdate reactive P in the leachate aqueous phase was also measured. See the methods section of the manuscript for more details.

Critical Details

1 – The source data from Grieger et al. (2022) that is used in this data package and associated manuscript is also used in Myers-Pigg et al. (2024a https://doi.org/10.1021/acs.est.3c10826; 2024b

https://data.ess-dive.lbl.gov/datasets/doi:10.15485/2327028) and Roebuck et al. (2025 https://doi.org/10.1016/j.scitotenv.2024.178040).

2 – Follow these step-by-step instructions to reproduce the figures and statistics for the manuscript associated with this data package:

1. Before getting started, download files from (Grieger et al., 2022; doi: 10.15485/1894135). Refer to "Barnes_2024_BSLE_P_Gradient/data/BSLE_Data_Package_v3/published_data_readme.md" for details on how to download and set up that data.
2. Open R and set the working directory to the folder where this readme file is located.
3. Open `BSLE_P_Code_for_Submitted_Manuscript_Revisions.Rmd` and run the code. *Note that all instances of saving the data frame and figures have been commented out.* If you would like to save these, please remove the #s from those lines of code.

3 – To rerun specific portions of the workflow:

- **Solid char ICP-OES** statistics and figures can be reproduced by downloading these data from Grieger et al. (2022), saving them in "data/BSLE_Data_Package_v3/v3_BSLE_Data" folder, and running the "BSLE_P_Code_for_Submitted_Manuscript_Revisions.Rmd" script.
- **Leachate ICP-OES (coarse filtered and < 0.7 µm filtered)** statistics and figures can be reproduced by downloading these data from Grieger et al. (2022), saving them in "data/BSLE_Data_Package_v3/v3_BSLE_Data" folder, and running the "BSLE_P_Code_for_Submitted_Manuscript_Revisions.Rmd" script.
- **Molybdate-reactive P** statistics and figures can be reproduced by downloading these data from Grieger et al. (2022), saving them in "data/BSLE_Data_Package_v3/v3_BSLE_Data" folder, and running "BSLE_P_Code_for_Submitted_Manuscript_Revisions.Rmd" script.
- **^{31}P NMR spectra** from Grieger et al. (2022) were further processed in MNova to identify and quantify chemical species. These results are included within this data package in the "P-NMR" folder. After downloading these data and saving within "data/Barnes_2024_BSLE_P_Gradient" folder, summary details and figures can be reproduced by running the "BSLE_P_Code_for_Submitted_Manuscript_Revisions.Rmd" script.
- **P XANES** from Grieger et al. (2022) were further processed in R and Athena (Ravel and Newville 2005) to identify and quantify chemical species. To recreate all additional processing steps:
    - Download data from Grieger et al. (2022) and save in "data/BSLE_Data_Package_v3/v3_BSLE_Data" folder.
    - Identify preliminary sample fits using the LCF package (Werner et al. 2017) in R to create a subset of reference compounds. Recreate this by running the "LCF_Package_P_Fits.Rmd" found within the "XANES_Determine_RC_Subset_for_LCF" folder. This script was run locally, so modify it to match your input and output folder structure. Applicable outputs to this manuscript are included in the "Athena_Code_Output" folder. These results were synthesized offline into a list of reference compounds to use in subsequent linear combination fits.
    - Import data ("P-XANES_Ref_Compd" and "P-XANES_Samples" folders) to Athena from "data/BSLE_Data_Package_v3/v3_BSLE_Data/BSLE_XANES" folder. Finalize the background subtraction and normalization parameters for samples and reference

compounds ("File_BS_Norm_Parameters.csv") and then perform linear combination fits. These results are published in this data package ("Barnes_2024_BSLE_P_Gradient/P-XANES" folder) within the "P_XANES_Reference_Compounds" and "P_XANES_Samples" folders.
    - Run the "XANES_Spectra_Merging.Rmd" script after saving the "P_XANES_Reference_Compounds" and "P_XANES_Samples" folders. This script processes normalized spectra so that it is in a figure-friendly format. Outputs of this script are published in this data package within the "P_XANES_Reference_Compounds" and "P_XANES_Samples" folders.
- To recreate only the **summary details** and figures used in the manuscript, run the "BSLE_P_Code_for_Submitted_Manuscript_Revisions.Rmd" script after saving data from this data package as "data/Barnes_2024_BSLE_P_Gradient".

Data Package Structure

This data package is comprised of a "data" folder and a series of data processing and analysis scripts. Details on how to recreate the workflow can be found in the Critical Details section of the readme and the "workflow_readme.md" file. The file-level metadata file (file ending in "flmd.csv") lists all files contained in this data package and descriptions for each. The data dictionary (file ending in "dd.csv") describes all tabular data columns and their respective definitions and units.

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.

To cite this data package:
Barnes M E ; Aronstein P J ; Bailey J D ; Bladon K D ; Forbes B ; Garayburu-Caruso V A ; Grieger S ; Graham E B ; McKever S A ; Myers C R ; Munson K M ; O'Day P A ; Powers-McCormack B ; Renteria L ; Roebuck A ; Scheibe T D ; Young R P ; Myers-Pigg A N (2024): Data and scripts associated with: "Burn severity and vegetation type control phosphorus concentration, molecular composition, and mobilization". River Corridor and Watershed Biogeochemistry SFA, ESS-DIVE repository. Dataset. doi:10.15485/2547035.

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Barnes ME; Roebuck A; Grieger S; Aronstein P; GarayburuCaruso VA; Munson KM; Young RP; Bladon KD; Bailey J; Graham EB; Renteria L; O'Day P; Scheibe TD; Myers-Pigg A (2025) Burn severity and vegetation type control phosphorus concentration, molecular composition, and mobilization. doi: 10.5194/egusphere-2025-21

Citations:

- Grieger S; Aronstein P; Bailey J Barnes M; Barton R; Bladon K D; Chu R; Forbes B; Garayburu Caruso V A; Graham E B; Goldman A E; Homolka K; Kew W; Lipton A S; McKever S A; Munson K M; Myers C R; Nieto-Pereira N; O'Day P; Otenburg O; Renteria L; Roebuck A; Scheibe T D; Torgeson J M; Toyoda J G; Wagner S; Young R P; Myers-Pigg A (2022) Organic matter concentration and composition of experimentally burned open air and muffle furnace vegetation chars across differing burn severity and feedstock types from Pacific Northwest, USA (v3). River Corridor and Watershed Biogeochemistry SFA, ESS-DIVE repository. Dataset. doi:10.15485/1894135.
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Change History

Change history:

Data Package Version	Changes
Version 1	Original data package publication

May 2025	