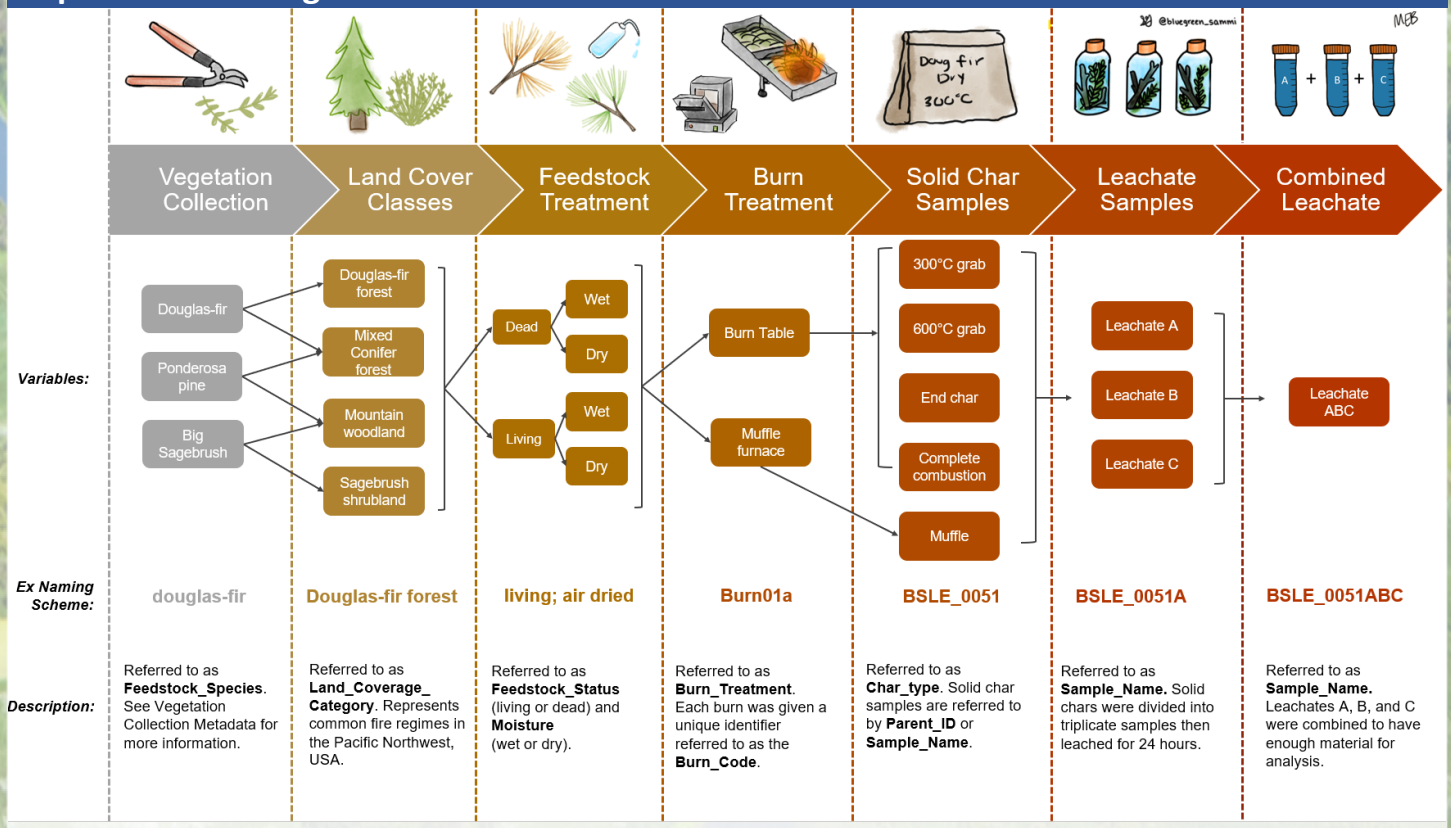
Title

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).

Summary

This dataset represents results from an experimental study designed to compare how the chemical composition of organic matter changes across different burn conditions and feedstock materials. The dataset provides both solid and dissolved phase bulk concentration and organic matter characterization data from experimentally generated chars. Chars were created in a closed muffle furnace or on an open burn table from four different feedstock species representing vegetation commonly impacted by fire regimes across the Pacific Northwest, USA. This data can be used to compare how different burn conditions may influence resultant organic matter chemistry and help further our understanding of potential biogeochemical impacts on river corridors post-fire.

Experimental Design



Vegetation Collection – Three plant species were collected for this experiment: douglas-fir, ponderosa pine, and big sagebrush. Metadata about the vegetation collection details can be found in BSLE_Vegetation_Collection_Metadata.csv. Douglas-fir and ponderosa pine were separated by living and dead material.

Land Cover Classes – Four land cover classes were constructed to represent commonly impacted fire regimes in the Pacific Northwest. The four categories were Douglas-fir forest, Mixed Conifer forest, Mountain woodland, and Sagebrush shrubland. The land coverage categories were made by homogenizing vegetation collected in the field before the burn.

Feedstock Treatment – Within land coverage categories, feedstock was separated by two treatment conditions: Feedstock_Status and Moisture. Feedstock_Status indicates if the vegetation material (Douglas-fir or Ponderosa pine) was living or dead when collected. Moisture indicates if the vegetation material was air-dried or if moisture was added. These conditions were manipulated to influence the fire fuel conditions, impacting the burn severity of the materials post-burn. These feedstock treatments are used as a proxy for vegetation type and/or landcover type and may be referred to as such in accompanying manuscripts.

Burn Treatment – In this experiment, 28 experimental burns were carried out. Half (14) were conducted in a closed muffle furnace while the other half (14) burns were conducted on an open-air burn table. Each individual experimental burn was assigned a Burn_Code. Char_Type indicates the type of solid char sampled during the burns and full definition can be found in BSLE_dd.csv. See BSLE_Burn_Protocol.pdf for any additional details about burn experimental design and execution.

Solid Char Samples – From the 28 burns, 69 unique solid char samples were generated. Each solid char sample was labelled with a unique Parent_ID (also called Sample_Name). The format for Parent_ID was "BSLE_####" in which #### is a 4-digit numeric code and spanned from BSLE_0001 to BSLE_0086.

Leachate Samples – For the leachate experiment, each solid char sample was weighed out into three 1-liter bottles to be leached in synthetic rainwater for 24 hours (see BSLE_Laboratory_Protocol.pdf for more information). To indicate a leachate sample, a letter was appended to the Parent_ID for each of the three leachates (e.g. A, B, or C). For example, the Sample Name of the leachate samples that came from solid char sample "BSLE_0001" are named "BSLE_0001A, BSLE_0001B, and BSLE_0001C" to indicate replicates.

Combined Leachate – Some analyses were run after combining the leachate replicates. This was done either because 1) sample volume was limited within the respective replicates or 2) we were limited in our ability to run all samples for the analyses and wanted to capture heterogeneity across replicates within a single Parent_ID. To indicate this, all letters of the leachates were appeneded to the Parent_ID. For example, the combined leachate sample that came from solid char sample "BSLE_0001" are named "BSLE_0001ABC".

Critical Details

1 – For analyte data, Sample Names are structured as "BSLE_0001A-filt0.2" where the descriptor appended to the Sample Name indicates the filtrate stage the data was analyzed at. A sample name with "-filt0.2" appended indicates it was filtered through a 0.7 micrometer filter and then a 0.2 micrometer filter. A sample name with "-filt0.7" appended indicates it was only filtered through a 0.7 micrometer filter. A sample name with "-unfilt" appended indicates the measurement was taken from unfiltered leachate water, and "-solid" refers to data collected on solid ground char. Any sample names with "Blank" are referencing blank 1-liter synthetic rainwater samples leached without any char in them. Blanks represent control samples for each day of the leaching experiment.

2 – Future versions of this data package will be published with additional datasets including: major anions and cations, compound specific isotopic values of 13C for benzene polycarboxylic acids (BPCA), nuclear magnetic resonance (NMR) for hydrogen, amino acid concentrations, anhydrosugar concentrations, X-ray absorption near edge structure (XANES) for nitrogen and carbons, and X-ray

photoelectron spectroscopy (XPS). This list is not exhaustive and additional analyses may be included in future releases of this data package.

3 – It is recommended that dissolved black carbon concentrations be calculated from individual BPCAs using the following equation described by Stubbins et al., 2015 (doi: 10.3389/feart.2015.00063): $[DBC] = 0.0891x([B6CA+B5CA])^{0.9175}$

4 – Post-processing scripts for binning the 13C-NMR data can be found at https://github.com/bpbond/nmrrr

5 – Spiking experiments were conducted for solution-state 31P-NMR data, where samples were spiked with known compounds to identify their chemical shift (ppm). These data column headers contain the sample name (i.e., BSLE_0001-solid) followed by an abbreviation for what compound(s) was/were spiked into the sample (i.e., alphaGP). Samples may have multiple columns of data to represent all spiking experiments and compounds added across multiple NMR experiments. The order of compounds listed indicates the order they were spiked into the sample. All compound abbreviations, the corresponding compound name, supplier, and molecular information can be found in "P-NMR_Spiking_Table.pdf".

Data Package Structure

This dataset is comprised of one data package readme, one data dictionary (dd), one file level metadata (flmd), fourteen burn table videos, burn table video metadata and three folders containing (A) data; (B) metadata and protocols; and (C) photos. The folder names of Folder A, Folder B, and the data package readme include a version number which will be updated with future iterations of this data package. Folder A includes (1) solid carbon and solid nitrogen; (2) dissolved organic carbon (DOC, measured as non-purgeable organic carbon, NPOC) and total dissolved nitrogen (TN); (3) pH; (4) thermocouple time series temperature; (5) methods codes; (6) installation methods; (7) excitation emissions matrix (EEM) methods information; and (8) a folder of excitation emissions matrix (EEM) fluorescence and absorbance spectra in dissolved organic matter and EEMs processing instructions; (9) solid state carbon-13 and solution state phosphorus nuclear magnetic resonance (13-C NMR and 31-P NMR) data and methods; (10) benzene polycarboxylic acid (BPCA) concentration data; (10) FTICR-MS methods; (11) Inductively coupled plasma (ICP) data for total calcium, magnesium, iron, aluminum, potassium, phosphorus, sodium, and sulfur along with sodium hydroxide-EDTA extractable calcium, magnesium, iron, aluminum, potassium, phosphorus, and sulfur; (12) a folder of phosphorus X-ray absorption near edge structure (P-XANES) data for samples and standards; (13) P-XANES methods; (14) molybdate reactive phosphorus; and (15) folder of high resolution characterization of organic matter via 21 Tesla Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS) generated through the Environmental Molecular Sciences Laboratory (EMSL; https://www.pnnl.gov/environmental-molecular-sciences-laboratory). The FTICR folder contains .txt data files and a subfolder containing instruments for using Formularity (https://omics.pnl.gov/software/formularity) and an R script to process the data based on the user's specific needs. Folder B includes (1) international geo-sample number (IGSN) mapping file (2) burn and laboratory metadata; (3) burn protocol; (4) laboratory protocol; (5) vegetation collection metadata; and (6) vegetation collection protocol. Folder C contains photos of the solid chars. All files are .csv, .txt, .pdf, .jpg, .jpeg, .R, .ref, or .mp4.

Citations and Acknowledgements

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FTICR-MS data were generated at the Environmental Molecular Sciences Laboratory, a DOE BER User Facility (EMSL; https://ror.org/04rc0xn13), under the EMSL User Proposal 51840.

Cite this data package with the appropriate DOI.

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Change History

Version 1	October 2022	Original data package publication
Version 2	April 2023	• Added 21T FTICR, solid state 13C-NMR, and BPCA data and associated methods information • Updated the readme, dd, flmd, and method code file to reflect changes
Version 3	September 2023	• Added solution state 31P-NMR, P-XANES, molybdate reactive phosphorus, and ICP data and associated methods information • Revised BSLE_NPOC_TN.csv. Original data used QAQC approach (blank correction) that has been removed. The unit basis was also updated for clarification. • Updated the 13C-NMR sample names to match other files in data package. Added an additional 0 (i.e. BSLE_### to BSLE_0###) • Updated the readme, dd, flmd, and method code file to reflect changes