

[10.1071/SR19396](https://doi.org/10.1071/SR19396)

Soil Research

Supplementary Material

Continental-scale measurements of soil pyrogenic carbon in Europe

Yamina Pressler^{A,}, Claudia M. Boot^B, Samuel Abiven^{C,D}, Emanuele Lugato^E, and M. Francesca Cotrufo^F*

^ANatural Resources Management and Environmental Sciences Department, California Polytechnic State University, San Luis Obispo, CA 93407, USA.

^BDepartment of Chemistry, Colorado State University, Fort Collins, CO 80521, USA.

^CLaboratoire de Géologie, UMR 8538, Ecole Normale Supérieure, CNRS, PSL Research University, Paris, France.

^DCentre de Recherche en Ecologie Expérimentale et Prédictive (CEREEP-Ecotron Ile de France), Département de Biologie, Ecole Normale Supérieure, CNRS, PSL Research University, Paris, France.

^EEuropean Commission, Joint Research Centre, Ispra (VA), Italy.

^FSoil and Crop Sciences, Colorado State University, Fort Collins, CO 80521, USA.

* Correspondence to: Yamina Pressler Natural Resources Management and Environmental Sciences Department, California Polytechnic State University, San Luis Obispo, CA 93407, USA Email: ypressle@calpoly.edu

Supplementary Material 1

Pressler, Y., Boot, C., Abiven, S., Lugato, E., Cotrufo, M.F. Continental-scale measurements of soil pyrogenic carbon in Europe.

We used Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) to acquire mid-infrared spectra from soil samples (n=397). Spectra were collected on a Thermo Scientific Nicolet iS50 Fourier Transform Infrared Spectrometer with a DRIFTS attachment. For each sample, we collected reflectance on 128 scans between 400 and 4000 cm^{-1} wavelengths at 4 cm^{-1} resolution. Uncorrected spectra for two soil samples are shown in Figure S1. See main text and Supplementary Material 2 for additional details on baseline correction and spectral pre-processing.

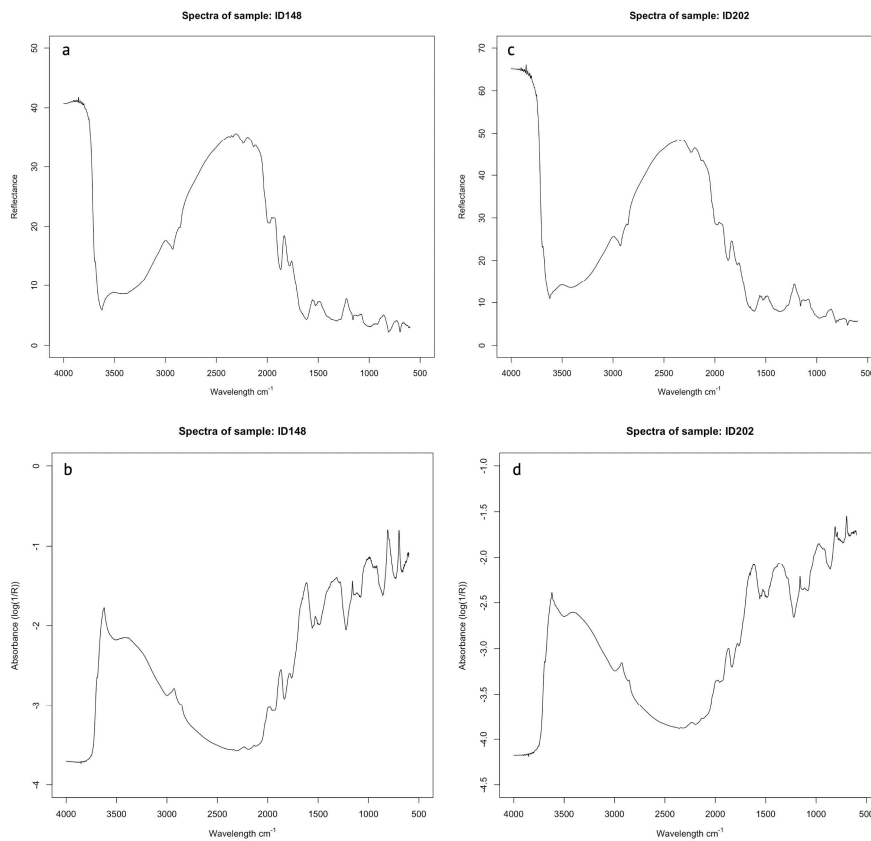


Figure S1. Unprocessed Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) spectra from select soil samples. Spectra are presented as Reflectance (a, c), and Absorbance (b, d).

Supplementary Material 2

Pressler, Y., Boot, C., Abiven, S., Lugato, E., Cotrufo, M.F. Continental-scale measurements of soil pyrogenic carbon in Europe.

DRIFTS spectra were pre-processed prior to PLS analysis. Spectra were first cut to only include the organic portion of interest (wavelengths $< 2500 \text{ cm}^{-1}$) and then rubberband baseline corrected. We then investigated several spectral pre-processing treatments to account for light scattering using the prospectr package (Stevens and Ramirez-Lopez, 2020) and EMSC package (Liland and Indahl, 2020) in R (Figure S2), including multiplicative scatter correction (MSC), extended multiplicative scatter correction (EMSC), and standard normal variate correction (SNV). We evaluated the extent to which spectral pre-processing for light scattering improved the PLS model (Table S2). Given that pre-processing did not improve the model (Table S2), we conducted the final analysis on the rubber band baseline corrected spectra only.

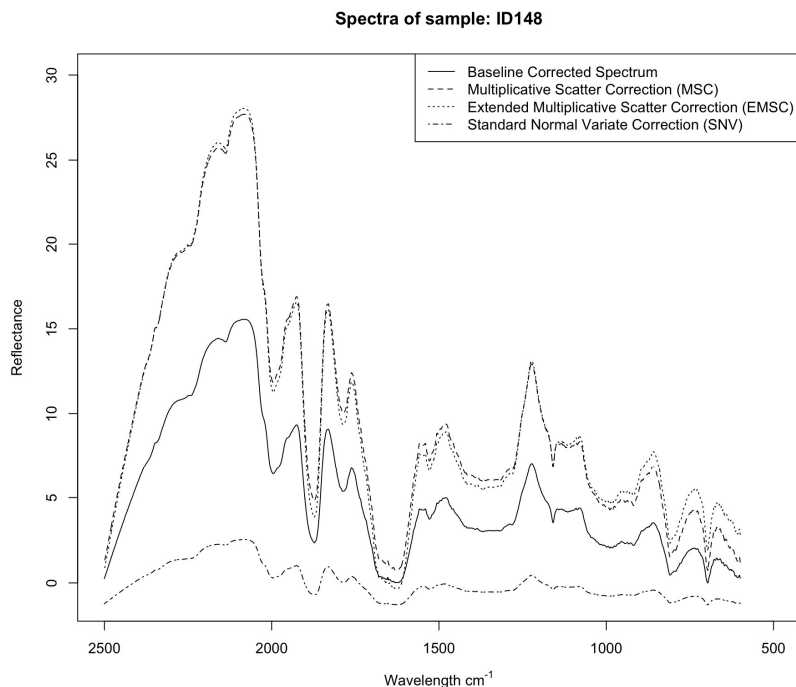


Figure S2. Example of DRIFTS spectral pre-processing for one soil sample. Prior to pre-processing

for light scattering, the spectrum was cut to include only the organic portion (wavelengths < 2500 cm⁻¹) and rubberband baseline corrected (solid line) with the hyperSpec package in R (Beleites and Sergio 2018). Then, spectra were pre-processed using multiplicative scatter correction (dashed line), extended multiplicative scatter correction (dotted line), or standard normal variate correction (dash-dot line).

Table S2. Comparison of DRIFTS spectra pre-processing treatments on PLS model performance. X- and Y-variance explained by the calibration model, R² of the calibration model, R² of the validation model, R², Root Mean Squared Error of Prediction of cross-validation (RMSEP), Ratio of Performance to Deviation (RPD; ratio of standard deviation to root mean squared error of cross validation) and number of latent variables are reported for each pre-processing treatment. Only results for the total BPCA-C model are presented, but results were similar for B6CA and B5CA models.

Pre-processing treatment	X-variance explained (%)	Y-variance explained (%)	R² calibration	R² validation	RMSEP	RPD	Number of Latent Variables
Rubber band baseline correction only	99.19	62.01	0.62	0.43	0.24	1.41	7
Multiplicative scatter correction	90.47	59.28	0.59	0.47	0.23	1.41	4
Extended multiplicative scatter correction	93.55	61.42	0.61	0.40	0.23	1.46	5
Standard normal variate correction	74.84	58.40	0.58	0.53	0.22	1.60	2

Supplementary Material 3

Pressler, Y., Boot, C., Abiven, S., Lugato, E., Cotrufo, M.F. Continental-scale measurements of soil pyrogenic carbon in Europe.

We used partial least squares (PLS) regression with the kernel algorithm and leave-one-out cross validation to calibrate the baseline corrected DRIFTS spectra to the BPCA-C data using the *pls* package in R (Mevik et al. 2016). X-loading values represent the contribution of different spectral regions to the predictive models. X-loading values of the PLS model for PyC-related spectral regions (aromatic carbonyl/carboxyl C=O, aromatic C=C, aliphatic C-O, and aromatic C-H) were low, suggesting that the model was not able to distinguish pyrogenic material.

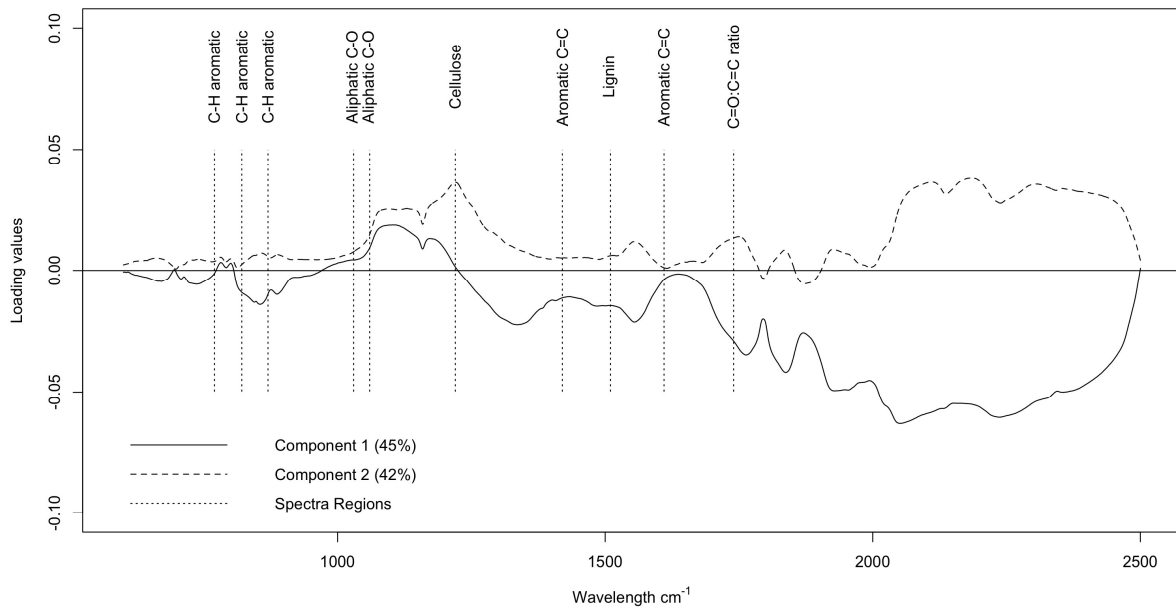


Figure S3. X-loading values representing contribution of different spectral regions to the total BPCA-C partial least squares regression model. Loading values for component 1 (solid line) and component 2 (dashed line) are shown. Spectral regions of interest are identified with dotted lines.