Scaling High-resolution Soil Organic Matter Composition to Improve Predictions of Potential Soil Respiration Across the Continental United States

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Key points:

- Molecular measurements of dissolved SOM are critical to accurately predict soil respiration at the continental scale.
- Machine learning extracts key molecules from complex high-resolution SOM profiles to explain differences in potential soil respiration.
- Dissolved SOM profiles provide more power in predicting potential respiration in surface soils than subsoils.

Abstract

Despite the importance of microbial respiration of soil organic matter (SOM) in regulating carbon flux between soils and atmosphere, soil carbon cycling models remain primarily based on climate and soil properties, leading to large uncertainty in predictions. With data from the 1000 Soils Pilot of the Molecular Observation Network (MONet), we analyzed high resolution water-extractable SOM profiles from standardized soil cores across the United States to address this knowledge gap. Our innovation lies in using machine learning to distill the thousands of SOM formula into tractable units; and it enables integrating data from molecular measurements into soil respiration models. In surface soils, SOM chemistry provided better estimates of potential soil respiration than soil physicochemistry, and using them combined yielded the best prediction. Overall, we identify specific subsets of organic molecules that may improve predictions of global soil respiration and create a strong basis for developing new representations in process-based models.

Plain Language Summary

Soil organic carbon (C) is one of the largest and most active pools in the global carbon cycle. Microbial decomposition of soil organic matter (SOM) releases large amounts of carbon dioxide (CO_2) to the atmosphere. This process is soil microbial respiration. To evaluate if SOM composition can improve predictions of soil respiration, we collected soils from across the continental US, and analyzed both soil physicochemistry and molecular SOM composition, as part of the Molecular Observation Network (MONet). We developed machine learning (ML) based workflow to extract key SOM signatures and used the SOM signatures to predict potential rate of soil respiration, compared to standard soil physicochemistry. The results suggested that SOM composition improved the prediction of potential soil respiration in surface soils, where most soil carbon is stored. In deeper soils, the model performance was not improved, possibly due to the greater importance of mineral-associated SOM. Our results identified key SOM molecules in predicting potential soil respiration and supported the significance of SOM dynamics in future development of soil carbon models.

Introduction

Soil respiration is estimated to release 60-100 Gt of carbon (C) to the atmosphere per year (Giardina et al., 2014; Jian et al., 2021), six to ten times as much C as released by fossil fuel combustion (~10 Gt C (Friedlingstein et al., 2022)). Microbial respiration of soil organic matter (SOM) is one of the most important contributors to soil carbon dioxide (CO_2) emissions and a critical link in the global C cycle (Graham & Hofmockel, 2022). With increasing temperatures under climate change, soil C repositories are vulnerable to increased rates of microbial respiration (Lei et al., 2021; Melillo et al., 2017; Nissan et al., 2023), which leads to positive feedbacks in global CO_2 emissions and temperature rises (Bond-Lamberty & Thomson, 2010). Despite decades of research, soil C fluxes remain one of the largest uncertainties in global climate predictions (Mark A Bradford et al., 2016; Crowther et al., 2016; Davidson & Janssens, 2006; Todd-Brown et al., 2014; Warner et al., 2019). Novel molecular measurements have recently been applied to identify SOM composition in an effort to understand molecular-scale processes and reduce these uncertainties (Bahureksa et al., 2021; Billings et al., 2021; Liang et al., 2019; Sanderman et al., 2021). Despite these efforts, the performance of soil C models with refined chemical pools can vary greatly due to the difficulty of simplifying highly complex SOM into discrete pools (Cotrufo et al., 2013; Robertson et al., 2019; Sulman et al., 2014).

The interplay of factors such as soil moisture, pH, nutrients, mineralogy, and SOM chemistry governs microbially-derived transformations of SOM (Amador & Jones, 1993; Ciais et al., 2014; Curiel Yuste et al., 2007; Falloon et al., 2011); but these relationships are difficult to constrain due to the amount of possible interactions between these variables (Billings & Ballantyne IV, 2013; Graham & Hofmockel, 2022). The most commonly used modeling approaches are based on Raich's model, which estimates respiration primarily as a function of temperature and water availability (Raich & Potter, 1995; Raich et al., 2002). Newer process-based models use additional physicochemical measurements to represent microbial and mineral processes. They incorporate SOM chemistry either through several discrete pools or through their thermodynamic properties (Kyker-Snowman et al., 2020; Waring et al., 2020; Wieder et al., 2018). With large spatiotemporal heterogeneity and limited availability of comprehensive and standardized measurements, accurate predictions of microbial SOM decomposition at regional-to-continental scales remain challenging (Mark A. Bradford et al., 2021).

A better understanding of SOM concentration, composition, and bioavailability may enhance our ability to predict soil C cycling through their controls on soil respiration and related enzymatic activities (Kyker-Snowman et al., 2020; Robertson et al., 2019; Song et al., 2020; Waring et al., 2020; Wieder et al., 2018). Yet, we have little ability to extract meaningful information from the thousands of molecules detected by state-of-science measurements. Variations in the bioavailability of chemical classes of SOM are mediated by geochemical and biophysical constraints, such as microbial biomass and necromass, reactive metals and minerals, organic and mineral horizon thickness, and other climate-related variables (Hall et al., 2020). For example, coarse-textured soil is more conducive to decomposition of chemically labile litter-derived C potentially due to higher fungal activity in organic-rich horizons (Huys et al., 2022; Scott et al., 1996). In addition, the interface between fresh litter inputs and soil minerals can serve as a hotspot for microbial breakdown of fresh C, resulting in the formation of soil aggregates and organo-mineral associations (Witzgall et al., 2021). This variability underlines the essential need to identify unique subsets of SOM that contribute more to soil respiration among different ecosystems and soil depths.

Although molecular measurements can provide unprecedented characterization of the thousands of individual formulae in SOM, data interpretation largely remains guided by coarse chemical and ecological groupings. Unsupervised machine learning models that summarize large data into lower-dimensional signatures have been widely used to study microbial ecology, SOM composition, and other environmental problems (Sonnewald et al., 2020). Here, we develop models using semi-supervised machine learning (non-negative matrix factorization with custom *k*-means clustering, NMF*k*) to reduce the complexity of molecular information into *k* distinct signatures of SOM chemistry from soils collected across the continental United States. NMF*k* leverages both the inherent structure of the data (through NMF, an unsupervised method) and domain knowledge guided signature determination (custom k-means clustering) to extract ecologically meaningful SOM signatures. We then explore the extent to which these signatures can provide additional insight into soil respiration beyond routinely collected variables. Our novel workflow results in a 1,000-fold decrease in SOM complexity, and the extracted SOM signatures can improve predictions of potential soil respiration ~~a~~cross soils from vastly different ecosystems. This enables data from state-of-science measurement techniques to be filtered into subsets of molecules that most directly explain soil respiration. Our workflow is applicable to multiple types of mass spectrometry data and to studies ranging from localized experiments to global surveys.

Methods

Soil sampling and characterization.

As part of the 1000 Soils Pilot study for the Molecular Observation Network (MONet), we collected 66 soil cores from across the continental United States (Figure S1), in collaboration with the U.S. National Ecological Observatory Network (NEON). MONet and NEON are continental scale programs that offer complementary open and standardized ecosystem data types. Standardized sampling procedures for soil core collection and analysis were previously described by Bowman et al. (2023). Briefly, two long cores (30 cm) and three short cores (10 cm) were collected at each site. Long cores were then divided into surface soil (0-10 cm) and subsoil (deepest 10 cm) and homogenized for further analysis. We also conducted field measurements, including soil temperature, volumetric water content, vegetation type, and weather conditions. Cores were shipped on ice overnight to the Pacific Northwest National Laboratory for further analysis. A full description of sampling and analytical methodologies are available in Text S1.

Water extractable SOM characterization.

We extracted water-soluble SOM from soils using solid phase extraction, and then analyzed extracts using a Bruker 7T Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS) at the Environmental Molecular Sciences Laboratory (EMSL) in Richland, WA. More details on SOM extraction methods and FTICR-MS analysis are in Text S1 and Bowman et al. (2023). Raw FTICR-MS data was processed with CoreMS (Python package, installed on 2022/11/22) (Corilo et al., 2021), including signal processing, peak detection, and molecular formula assignment (Text S1). We predicted compound classes of the filtered formulae based on O/C and H/C ratios of van Krevelen classes (Kim et al., 2003; Tfaily et al., 2015). The suffix "-like" in chemical classes, such as "lignin-like", indicates the uncertainty of the van Krevelen classification method (Tfaily et al., 2015). We converted the peak intensity values to present/absent (1/0) and separated the final dataset by soil depth (surface vs. subsoil) for statistical analysis. Alpha diversity was calculated as the total number of formulae identified in each sample (i.e., richness).

Data analysis and machine learning methods.

We used linear regression models to evaluate the relationship between potential soil respiration and soil physicochemical variables (Text S3). To avoid potential biased relationships from different magnitudes of the data, we performed $\log_{10}$ transformation on potential respiration rates, total C, total N, total sulfur, and Mn concentration.

We used NMF*k* (Bhattarai et al., 2020) to identify SOM signatures from the 7312 and 5515 SOM formula detected by FTICR-MS (for surface and subsoil, respectively) with *pyNMFk* package (Python, https://github.com/lanl/pyDNMFk, Figure 1). More details on NMF*k* assumptions, model settings, and model robustness are in Text S2. Briefly, NMF*k* tends to be more successful at extracting explainable basis or signatures from large multivariate datasets, compared to other dimensionality reduction tools such as principal component analysis (Devarajan, 2008; D. Lee & Seung, 2000). As applied here, NMF*k* summarizes data into discrete signatures that contain weights for each SOM formulae for each soil layer independently (i.e., a separate set of signatures was generated for surface versus subsoils to explore depth-specific relationships). The optimal number of signatures was determined from silhouette coefficients. A W-matrix with the weights of each SOM formulae (*N*) to each extracted signature (*k*), and an H-matrix with the contribution of each signature (*k*) to each soil sample (*m*) were generated from NMF*k*.

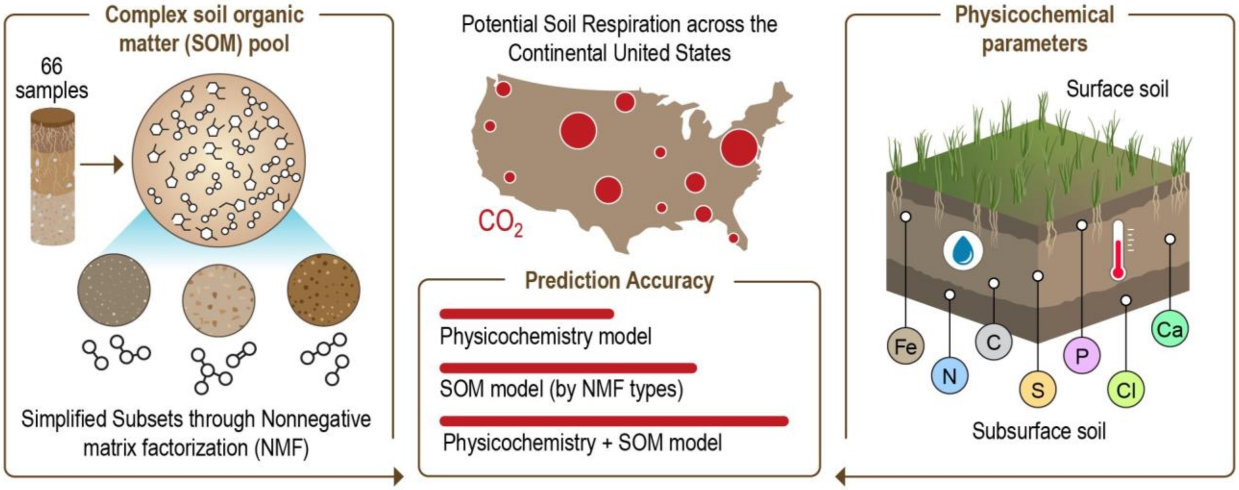

Figure 1. Workflow: Machine learning models summarize SOM composition to predict potential soil respiration. NMFk extracts key SOM signatures from high resolution mass spectrometry measurements of SOM. Gradient boosting regression predicts potential soil respiration with physicochemistry, SOM signatures, and physicochemistry combined with SOM signatures.

To define levels of potential soil respiration, we used *k*-means clustering with the elbow method to select the number of groups (*KMeans* from *scikit-learn* package, Figure S2) (Bholowalia & Kumar, 2014). Then, we mapped the extracted *k* signatures to potential soil respiration using supervised machine learning. To evaluate the value of NMF*k*-extracted signatures for explaining soil respiration, we conducted three sets of machine learning models: (1) selected physicochemical variables alone (i.e., variables with $r^2 > 0.2$ in individual regression, Table S1), (2) SOM signatures alone (NMF*k* weights from H-matrix), and (3) physicochemical variables and SOM signatures combined. All machine learning models were built using gradient boosting regression (GBR) from *scikit-learn* package (v 0.24, Python). More details on model training, testing, and validation are in Text S3.

Results

Soil physicochemistry and potential respiration

Overall, many soil parameters, including potential soil respiration, tended to be higher in surface soils than in subsoils. Significant differences ($p < 0.05$) between surface soils and subsoils in total C, total N, total sulfur, C/N ratio, and other factors are shown Figures S3 and S4. In particular, surface soils had higher potential respiration rates (median: 72.6 ug CO_2/g soil/day) than subsoils (median: 21.9 ug CO_2/g soil/day) (Figure S3(a), Mann–Whitney U = 3022.5, $N_{surface} = 63$, $N_{subsoil} = 61$, $p < 0.05$).

For both surface and subsoils, soil with high potential respiration tended to be sourced from the Midwestern and Northeastern United States. (Figure S5). In surface soil, high potential respiration was associated with five soils collected in Utah, Wyoming, and Virginia (within temperate conifer forest and temperate broadleaf & mixed forest biomes, Figures S1, S5). In subsoils, high respiration was associated with three soils from Utah and Maryland (temperate conifer forests and broadleaf & mixed forests biomes). Desert soils had the lowest respiration in both layers (Figure S1).

We found relationships between soil respiration and many physicochemical variables that supported prevailing paradigms (Figure S4, associated discussion in Text S4). A full correlation table is available in Table S1. Briefly, potential respiration rates in both surface and subsoils were positively correlated with gravimetric water content (GWC) ($r^2 = 0.246$ and 0.225) and cation exchange capacity (CEC, $r^2 = 0.405$ and 0.354). They were also positively correlated with total C and total N content, with stronger relationships in surface soils ($r^2 = 0.487$ vs. 0.268 for total C, $r^2 = 0.439$ vs. 0.248 for total N). Total bases and magnesium (Mg) concentrations had a higher correlation to potential respiration in subsoils than surface soils ($r^2 = 0.227$ vs. 0.146 and 0.287 vs. 0.160), while manganese (Mn) concentrations were correlated to potential respiration in surface soils (r^2: 0.324).

SOM composition and NMFk partitioning of SOM.

Across all soils, the most common chemical classes of SOM were lignin-, condensed hydrocarbon-, and tannin-like formula. Most formula in these classes were present in both surface and subsoils (i.e., ‘shared’ formula). However, surface soils contained more unique formula than subsoils for all compound classes (Figure S5(c)). In particular, many protein-, amino sugar-, and lipid-like compounds were identified in surface soils only, with very few compounds in these classes being unique to subsoils. Soils from the Midwestern U.S. and the West Coast had relatively higher alpha diversity than soils from other regions (Figure S5(a)).

Then, we used NMF*k* to summarize SOM composition into 7 and 5 NMF*k* signatures, respectively, for surface and subsoils (Figure 2). Geographic patterns in SOM signatures are displayed in Figure S6-7, with more geographic clustering of NMF*k*s in surface soils than in subsoils. The most important formula contributing to the composition of each NMF*k* (i.e., formula with normalized weights >0.5 in W-matrix) are shown in Figure 2(a-b). NMF*k*-selected formula (weights >0.5 in W-matrix) generally followed the same general patterns as the overall SOM pool but showed amplified relationships (Figure 2(c)).

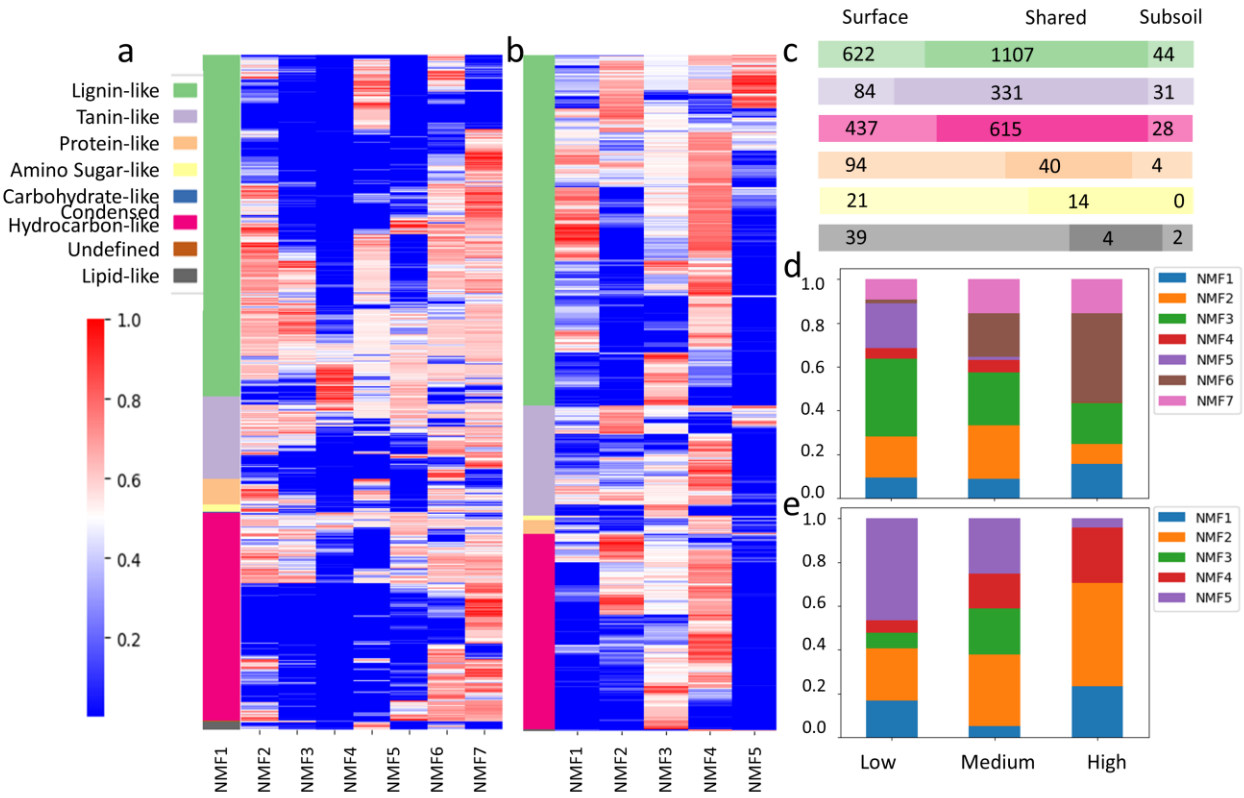

Figure 2. NMFk partitioning of SOM composition. (a-b) Relative contribution of SOM formula to each SOM signature identified by NMFk in a) surface and b) subsoils. The color (blue to red) in each cell represents the normalized (0 to 1) relative contribution for each SOM formula (row) to each NMFk signature (column). The left bar indicates the compound class of each SOM formula. (c) The number of shared and unique formula identified as important (normalized weights >0.5) by NMFk in surface and subsoils. (d-e) The relative contribution of NMFk signatures to each level of potential respiration in both d) Surface soils with potential respiration levels of low (N=44), medium (N=14), high (N=5) and e) subsoils with potential respiration levels of low (N=48), medium (N=10), high (N=3).

For surface soils, NMF1, 4, 6, and 7 had a relatively high number of important compounds identified as lignin-like. NMF6 and 7 had large contributions of condensed hydrocarbon-like formula. NMF1 had high contribution from protein-like and amino sugar-like compounds, while NMF3 and 5 had the lowest contribution from protein-, amino sugar-, and lipid-like compounds of any NMF*k*. NMF4 had the largest number of lipid-like compounds as important features relative to any other surface soil NMF*k*s.

In subsoil samples, important formula for all NMFs tended to be classified as lignin-, tannin-, and/or condensed hydrocarbon-like. NMF1 and NMF5 had a larger fraction of features identified as lignin-like compounds than other NMF*k*s in subsoils. NMF2 and NMF3 had a larger fraction of condensed hydrocarbon-like compounds than other NMF*k*s, while NMF4 had large contributions of protein-like and amino sugar-like formula (Figure S8).

We also observed differences in the dominant NMF*k* signatures across high-, medium-, and low-respiration soils, particularly in surface soils (Figure 2(d-e)). High respiration surface soils were characterized by five NMF*k* signatures (1, 2, 3, 6, and 7), with the largest contribution from NMF6. Low respiration surface soils, in contrast, uniquely contained NMF5, and no contribution from NMF6. In subsoils, high respiration soils had high contribution of NMF3 and 4, while low respiration soils were disproportionately associated with NMF5.

Relative importance of physicochemistry and SOM composition in potential soil respiration models

We developed potential soil respiration models with (1) physicochemical variables, (2) NMF*k*-extracted SOM signatures, and (3) both of them combined. Model performances are summarized in Table S2 and Figure 3.

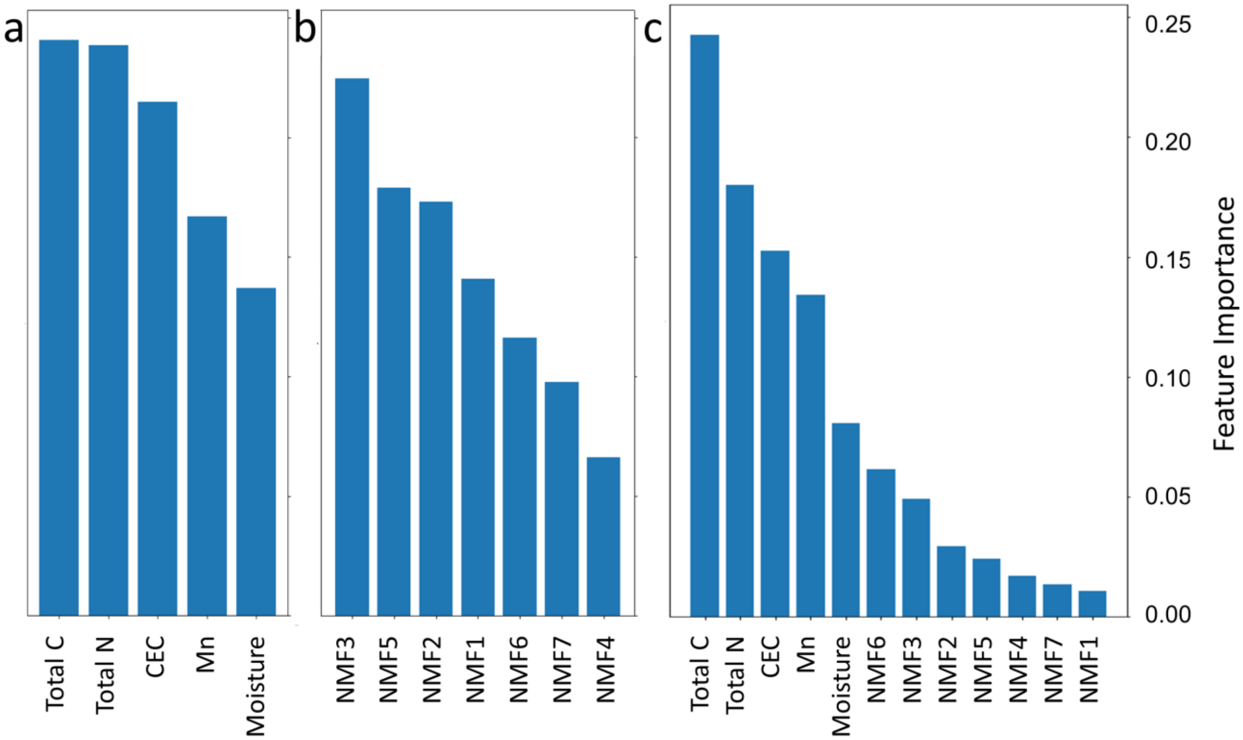

Figure 3. Relative importance of each predictor in surface potential soil respiration models. A) Model with physicochemical variables only. B) Model with SOM signatures only. C) Model with both physicochemical variables and SOM signatures.

Selected physicochemical variables (consisting of total C, total N, CEC, moisture, Mn (surface), total base (subsoil), and Mg (subsoil) concentration) had significant independent Pearson's correlation to respiration w/ $p < 0.05$ and $r^2 > 0.2$ (Table S1). Physicochemical variables predicted potential respiration rates in surface and subsoils equally well ($r^2 = 0.44$ and 0.43 respectively for testing data). In surface soils, total C, total N, and cation exchange capacity (CEC) were identified as the top 3 most important predictors, followed by Mn concentration and soil moisture (Figure 3). In subsoils, CEC, total N, and soil moisture were the most important predictor, and total C was the least important predictor (Figure S9).

Using NMF*k* signatures as predictors, we had better model performance in surface soils than in subsoils (testing $r^2 = 0.54$ vs. 0.08), and SOM signatures alone predicted slightly more variation in potential respiration rates than physicochemical variables alone in surface soils (testing $r^2 = 0.54$ vs. 0.44), even when controlling for an equal number of predictors (testing $r^2 = 0.48$ vs. 0.44). NMF3, NMF5, and NMF2 were the most important SOM composition variables for explaining surface soil respiration (Figure 3).

When we combined both physicochemical variables and SOM signatures into a single predictor set, we obtained better respiration model performance ($r^2 = 0.62$) compared to models with environmental variables or SOM signatures in surface soils only. However, the model describing potential respiration rates in subsoil was worse ($r^2 = 0.36$) when compared to models based on physicochemical variables only. In surface soils, the 3 most important variables were the same in the full model as in the physicochemical model. NMF6 was identified as the most important SOM variable, followed by NMF3, NMF2, and NMF5 (Figure 3).

Discussion

Depth partitioning in relationships between SOM composition and potential soil respiration

Regardless of depth or geographic location, the diversity of water-extractable SOM compounds appeared to be a common factor in regulating potential soil respiration — soils with higher potential respiration generally had more diverse pools of water-extractable SOM (Figure S5(e-f), Text S5). Yet, different subsets of SOM were disproportionately associated with soils exhibiting high vs. low potential respiration rates, as NMF weightings varied substantially across soils with different rates of potential respiration in both layers (Figure 2(d-e), Figure S6-S7).

Overall, our results were consistent with a paradigm in which chemically bioavailable, plant-derived molecules including proteins and amino sugars are degraded through soil profiles and transformed into microbially-derived byproducts that are subsequently stabilized via organo-mineral associations (Kallenbach et al., 2016; Roth et al., 2019; Zhao et al., 2020); whereas more chemically recalcitrant compounds (e.g., lignin and tannin) are preserved due to their lower thermodynamic bioavailability (Kögel-Knabner, 2002; Kramer & Gleixner, 2008; Rumpel & Kögel-Knabner, 2011). Coincident decreases in SOM diversity from surface to subsoils were also associated with decreases in potential soil respiration (Figure S5(d)), further supporting a link between SOM pool composition and microbial decomposition (Davenport et al., 2023; Kramer & Gleixner, 2008).

In more detail, surface SOM chemistry, as partitioned by NMF*k*, provided unprecedented resolution into the specific chemistries associated with prevailing paradigms in soil C cycling. Molecular formula in NMF6 especially displayed a dramatic increase in weighting from low-to-high respiration soils, putatively signaling a close relationship with elevated potential soil respiration. NMF6 contained a diverse suite of compounds including protein-, (soluble) lipid-, and amino sugar-like formula that can be rapidly used as microbial substrate. Proteins and amino sugars in particular can bolster microbial metabolism of SOM (Campbell et al., 2022; Hernández & Hobbie, 2010). Thus, the prevalence of these compounds within NMF6 may support high potential soil respiration. NMF1 and NMF7 also contained a diverse mixture of compounds and increased from low-to-high respiration soils, further supporting a relationship between SOM pool diversity and microbial respiration.

In contrast, NMF2, NMF3 and NMF5 in surface soils decreased in importance as potential respiration increased and primarily consisted of a small but unique subset of lignin- and tannin-like compounds (Figure 2(a)). This is consistent with low bioavailability of the chemical constituents of these NMFk's suppressing microbial respiration (Kögel-Knabner, 2002; Marschner & Kalbitz, 2003). It suggests that despite the often-inferred high bioavailability of water-extractable SOM (Garayburu-Caruso et al., 2020), there may be a significant fraction of SOM that is chemically protected from microbial decomposition (Garayburu-Caruso et al., 2020; Hernández & Hobbie, 2010; Tureţcaia et al., 2023). Lastly, NMF4 in surface soils — which contained the greatest number of lipid-like formula (Figure 2(a)) and had a comparatively large fraction of protein-like formula — was not present in any high-respiration soils. We therefore suggest that NMF4 may be an indicator of non-living microbial biomass (i.e., necromass) which is disproportionately comprised of lipids (microbial cell wall remnants) and amino sugars and proteins (the basis of intracellular materials) (Angst et al., 2021; Camenzind et al., 2023).

The distillation of multidimensional SOM composition profiles into a tractable set of molecules associated with soil respiration is a major obstacle in understanding soil C cycles (Billings et al., 2021; Garayburu-Caruso et al., 2020; Graham et al., 2018; Tureţcaia et al., 2023). The SOM formula within NMF*k*s that correspond to changes in soil respiration represent a key step forward in understanding the chemical bioavailability of water-extractable SOM, as it allows us allows us to downscale from the thousands of molecules detectable by state-of-science methods into more tractable units for further investigation. Our approach can be used with multiple different extraction types and/or high-resolution mass spectrometry measurements. Our results are particularly promising for surface soils, where the dissolved SOM pool (e.g., water-extractable SOM) is thought to fuel microbial respiration. The comparatively weak relationship between subsoil water-extractable SOM and potential soil respiration as compared to surface soils highlights recent work emphasizing the importance of mineral-associated organic matter in soil C storage (Benbi et al., 2014; Cotrufo et al., 2019; Lugato et al., 2021). We therefore suggest that combining our analytical workflow with measurements on mineral-associated organic matter specifically would increase our understanding of SOM cycling in deeper soils. An extended discussion of the relationships between SOM chemistry and potential soil respiration is available in Text S5.

Relative importance of physicochemistry and SOM composition in predicting potential soil respiration

Next, we parsed the contributions of physicochemistry and SOM composition (NMF*k*s) separately and in combination to predict potential rates of soil respiration using machine learning models. The models based on physicochemistry alone explained a modest amount of variation in soil respiration (44% and 43% in surface and subsoils, respectively), in line with the range of explanatory power observed in other works (Allison, 2012; Graham et al., 2014).

For surface soils, models based on SOM composition alone (54% variation explained) and both physiocochemical factors and SOM composition combined (62% variation explained) suggest that SOM composition (1) can predict soil respiration at least as well as commonly measured physiocochemical variables and (2) explains some portion of soil respiration that is not captured by physiocochemistry. While physicochemical predictors were stronger predictors of soil respiration than SOM composition in the combined surface soil model, the inclusion of SOM composition improved accuracy by 18% from the physicochemistry model, indicating that it may significantly impact our predictions of soil C cycling processes. NMF3 (which was mainly in low-respiration soil and was comprised of lignin- and tannin-like formula, see previous section) in particular was the strongest predictor of soil respiration in models based on SOM composition alone followed by NMF2 and NMF5. The relative chemical recalcitrance of the most important predictors of respiration may suggest that the proportion of thermodynamically unfavorable formula in water-extractable SOM has a direct inhibitory effect on soil metabolism. Indeed, thermodynamic regulation of organic C composition can be a key control for the rate of respiration in ecosystems (Garayburu-Caruso et al., 2020; Tureţcaia et al., 2023). NMF6, which was the most important NMF*k* signature in the combined surface soil model, consisted of diverse chemically-bioavailable compounds, and it mainly existed in high-respiration soils (Marschner & Kalbitz, 2003). We therefore suggest that chemically-bioavailable compounds in water-extractable SOM pools may provide the greatest complementary explanatory power to physicochemical factors in soil respiration predictions.

However, subsoil models displayed different dynamics. In the subsoil model with physicochemical variables alone, total C was the least important predictor (vs. the most important predictor for surface soils), and the model containing SOM composition did not yield high predictive power. The partial dependence of potential soil respiration to total C was stronger in surface soil than in subsoil (Figure S10), which could explain why SOM composition did not add predictive power to potential respiration in subsoils. Since more total and organic C is stored in surface soils, resolution into the water-extractable SOM pool (reflected here by NMFs) might be a more significant factor for predicting surface soil respiration than in subsoils, where there are lower total C and more mineral-associated SOM (Rumpel & Kögel-Knabner, 2011).

Conclusion

Leveraging SOM chemistry to improve conceptualizations and models of soil C cycling is a major opportunity in advancing global biogeochemical and climate predictions. In this study, we use machine learning (NMF*k*) to distill the thousands of SOM molecules detected by ultrahigh resolution mass spectrometry into tractable units associated with microbial respiration. Our results suggest that NMF*k*-extracted SOM signatures can improve surface soil respiration model performance by integrating fundamental molecular information across very different soil ecosystems. Because SOM pools vary tremendously at the continental-scale, refined regional or local studies that encompass lower-variability parameter spaces may yield even more value of SOM molecular data to soil C modeling. The chemical properties of SOM molecules represented by NMF*k* signatures agree with the contemporary understandings of SOM bioavailability and soil respiration. Furthermore, our workflow provides a basis for molecular information to spur the development of new process-based soil C cycling models and underscores the role of specific chemical constituents within the water-extractable SOM as determinants of soil respiration.

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Geophysical Research Letters

Supporting Information for

Scaling High-resolution Soil Organic Matter Composition to Improve Predictions of Potential Soil Respiration Across the Continental United States

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Introduction

The supporting information includes extended methods (Text S1, Text S2, and Text S3) and extended interpretation of results (Text S4 and Text S5). The extended methods sections provide extra details of analytical methods, data processing methods, and justifications. The extended results summarize the holistic relationships between soil physicochemistry, potential soil respiration, and SOM composition. The supporting figures (Figure S1 to S10) and supporting tables (Table S1 to S3) provide detailed findings referenced in the main manuscript and supporting text. All the data used in this study is publicly available on Zenodo at https://zenodo.org/records/10888508.

Text S1. Soil physicochemistry and SOM composition analysis

Per the methods outlined by Bowman et al. (2023), we divided 30-cm soil cores collected from around the continental United States into three 10-cm intervals, where only the top 10-cm (hereafter, surface soil) and bottom 10-cm (hereafter, subsoil) sections were used for further analysis. We mixed the top sections with three short cores (10-cm soil cores sampled at the same time and location) to homogenize any local variation in soil physicochemistry and SOM composition. The soils from each sampling interval were then sieved through 4 mm sieves to remove rocks and root structures. We then measured gravimetric water content (GWC) by drying 10 g of soil for 24 hours in a drying oven at 100 ^{0}C. We measured soil pH by mixing 20 g of dry soil with 20 mL of DI water (1000 rpm on reciprocating shaker for 15 minutes) and testing with a calibrated pH probe. Soil microbial biomass C and nitrogen (N) content were measured via chloroform fumigation (Brookes et al., 1985; Witt et al., 2000; Zhao et al., 2022). We extracted phosphorus contents using Bray (pH < 7) or Olsen extractions (pH > 7) (Bray & Kurtz, 1945; Corbridge, 1980), and we extracted nitrate and ammonium with 0.5M K_2SO_4 and tested by colorimetric methods. Ion concentrations of potassium (K), calcium (Ca), magnesium (Mg), and sodium (Na) from 1:10 ammonium acetate extraction, Zinc (Zn), manganese (Mn), copper (Cu), iron (Fe), boron (B), and sulfate (SO_4^{2-}) from 1:2 soil to diethylenetriaminepentaacetic acid (DPTA) extraction were measured using Inductively coupled plasma mass spectrometry (ICP-MS). We measured total C and N using the AOAC official methods 972.43 (AOAC, 2006). Soil texture was measured by hydrometer analysis. Finally, we assessed potential soil respiration using the CO_2 burst method with 24 hours of incubation at 24 ^{0}C (Bowman et al., 2023).

We extracted water-soluble SOM by mixing 6 g of dry soil with 30 mL DI water in triplicates, shaken for 2 hours at 800 rpm, and centrifuged at 6,000 rpm for 8 minutes. 5 mL of supernatant was acidified with 2 μL concentrated phosphoric acid (37%), and then loaded onto Agilent Bond Elut PPL solid phase extraction cartridges (Dittmar et al., 2008) with Gilson ASPEC® SPE system. A Bruker 7-T Fourier transform ion cyclotron resonance mass spectrometry (FTICR MS) at the Environmental Molecular Sciences Laboratory (EMSL) in Richland, WA, was used to analyze SOM composition, with a negative ionization mode and ion accumulation time at 0.01 or 0.025 seconds (depending on dissolved organic C concentration). The measured mass accuracy was typically within 1 ppm. One lab blank and one Suwannee River Fulvic Acid (SRFA) sample (20 ppm) were tested every 30 samples (randomized triplicate samples for both surface soil and subsoil at each site) to evaluate instrument performance.

We used CoreMS (https://github.com/EMSL-Computing/CoreMS) to process raw FTICR-MS data in Python. Noise thresholding was performed with signal-to-noise threshold (5 std.), mass error (0.3 ppm), and stoichiometric limits from domain knowledge (C: 1-90, H: 4-200, O:1-23, N: 0-3, S: 0-2, P: 0-1). SRFA standards were used to set a calibration threshold for all soils in the same batch. Molecular formula was assigned based on both accurate mass and filtered by their confidence score from CoreMS. After calibration and formulae assignment, we filtered the assigned peaks by *m/z* between 200 to 1,000, present in at least 2 out of 3 replicates, not present in two or more lab blanks, and with formulae confidence scores (combines *m/z* error and isotopic pattern) above 0.7 (Corilo et al., 2021).

Text S2. NMF*k* model assumption and model selection

We used NMF*k* to decompose the SOM composition matrix into multiple basis signatures, due to its ability to capture unique and sparse patterns from complex data (D. Lee & Seung, 2000). The underlying assumption of NMF*k* is that there are similar distributions of variables (SOM formula in this study) across samples, such that the main characteristics of each sample can be represented by the combination of a limited number of non-negative basis components (signatures) (Paatero & Tapper, 1994). It has also been widely used in environmental forensics (Johnson et al., 2015; Rodenburg et al., 2011), text mining (Pauca et al., 2004), and face recognition (Guillamet & Vitria, 2002). For example, Vesselinov et al. (2018) used NMF*k* to identify unknown sources of groundwater recharge driven by various physical and chemical processes; while Cai et al. (2017) used NMF to extract key features and reveal temporal patterns in microbial communities. Instead of relying on linear data transformations like principal components analysis (PCA), NMF*k* uses non-negativity constraints that makes it better suited to identify representative SOM signatures and evaluate their distribution in diverse samples. Furthermore, the additive fashion of extracted signatures to represent SOM composition by NMF*k* fit the intuition of different pools of SOM molecules adding up to the combined mixture of SOM in a certain sample. Therefore, the NMF*k* extracted SOM signatures are more explainable compared to PCA or other ordination techniques.

The number of signatures (k) was determined by k-means clustering coupled to a silhouette coefficient with a threshold of 0.5 to evaluate model stability (Bhattarai et al., 2020; Vangara et al., 2021). We evaluated a range of k from 2 to 20 for both models (surface soil and subsoil), where the highest k-model above the threshold (> 0.5) was selected as the final model. These criteria were chosen because the selected model should have good separation (more separation with a larger k) between different non-negative signatures but also a stable solution (above the threshold of silhouette coefficient) at the same time. To visualize the composition of each NMF*k* signature (W-matrix), we generated a heatmap of SOM formula with normalized weights (0-1) >0.5 in at least one NMF*k*, clustered by van Krevelen class assignment (*clustermap* function from *seaborn* package, v 0.12.1). We further clustered SOM formula by Van Krevelen classes using the "linkage" method from the *scipy* package (v 1.11.4, "ward" method with "Euclidean" distance) to illustrate the difference between NMF*k* signatures.

Text S3. Gradient boosting regression model development

Gradient boosting is a machine learning algorithm that combines multiple weak models, such as decision trees, iteratively to construct a stronger model, where each weak model learns from the residual error from the previous model (Friedman, 2001). It is one of the most powerful and effective machine learning models that is widely used in many different areas. Using an ensemble method, gradient boosting regression is capable of generating predictions from multiple decision tree models and thus provides a more robust prediction than individual decision trees. It usually has better performance with smaller datasets, because it is less likely to overfit the data (Hastie et al., 2009). Therefore, it is suitable for predicting soil respiration with physicochemistry and NMF*k* extracted SOM signatures.

We performed feature selection on physicochemical factors by statistical relevance (Table S1) to remove variables with little to no correlation to potential soil respiration, which likely introduce noise and can lead to model overfitting (Christ et al., 2018; Yuan et al., 2019). *stats.linregress* function from *scipy* package (v 1.11.4) in Python (v 3.7.1) was applied to calculate the fitted line, r^2 value (the square of *rvalue*, Pearson correlation), and p-value (*pvalue*). Pairwise plots with regression fitting were generated by the pairplot function from the *seaborn* package (v 0.12.1) in Python. Total C, total N, CEC, Mn and soil moisture were selected as predictors for surface soil models. Total C, total N, total base, CEC, Mg and soil moisture were selected for subsoil models.

Model hyperparameters were tuned first with 5-fold cross validation on 80% of soils in each dataset (*train_test_split* in scikit-learn, with the same *random_state* for models in the same layer) using *RandomizedSearchCV* function from scikit-learn. We then used the best-tuned parameters with 80% of soils to build the finalized model. Root means square error (RMSE) was used to evaluate the error of models. Detailed settings of the hyperparameter dictionary for *RandomizedSearchCV* and the best-tunned parameter set used for the final model are shown in Table S3. All the models were then tested with the other 20% of soils to compare their performance. The feature importance of each predictor was determined using MDI importance (mean decrease in impurity) to infer potential relationships between soil physicochemistry, SOM composition, and potential soil respiration. Partial dependence plots were used to evaluate the sensitivity of potential soil respiration in response to selected predictors (Figure S10).

To avoid the impacts of the increased number of predictors on improved model performance for surface soils (physicochemistry model: n = 5, SOM model: n = 7), we developed another version of SOM model without the two least important predictors (NMF7, NMF4). The model performance was still better (testing $r^2 = 0.48$ vs. 0.44) compared to the physicochemistry model with the same number of predictors ($n = 5$).

Text S4. Potential soil respiration and physicochemistry

Soil moisture, total C, and total N appeared to regulate potential soil respiration in both surface soil and subsoil, as evidenced by positive correlations of total C, N, and moisture with potential soil respiration (Figure S4). This is consistent with previous work describing relationships between these properties and soil respiration, as well as other factors that we observed to be correlated with potential soil respiration including pH and CEC (Chen et al., 2014; K.-H. Lee & Jose, 2003; Riaz & Marschner, 2020; Waring et al., 2020). Soil physical properties (e.g., moisture and pore space connectivity) can constrain microbial access to SOM molecules and nutrients isolated in soil pore networks, thereby regulating microbial respiration of SOM (Falloon et al., 2011; Moyano et al., 2013; Orchard & Cook, 1983; Waring et al., 2020; Xu et al., 2004). Additionally, C and N can limit soil respiration through stoichiometric constraints on biomass production (Elser et al., 2000; Graham & Hofmockel, 2022; Soong et al., 2020; Wang & Houlton, 2009). Notably, field temperature was not correlated with potential soil respiration in this study (Figure S4(h)). We posit this lack of relationship is due to the standardization of potential soil respiration assays, in which all respiration rates were measured at a common temperature. Future work to extend the methods applied here to field-based estimates of microbial respiration is a promising avenue to further constrain microbial respiratory pathways relevant to soil carbon cycling.

We propose that differences in potential respiration between surface and subsoil may be related to variation in soil C composition and stabilization mechanisms across soil layers. We observed a steeper correlation between total C and potential soil respiration in surface soils than in subsoils (Figure S4), despite similar slopes for relationships of N and moisture with respiration at both layers. While we anticipated that microbial respiration would decrease significantly with soil depth (Changming Fang & John B. Moncrieff, 2005), the change in the nature of the relationship between C and respiration suggests that differences in SOM composition or microbial access to C substrates could be associated with potential rates of respiration. Surface soils are generally rich in relatively bioavailable water-extractable organic matter and contain higher proportions of microbial biomass in contrast to subsoils that are more mineral with lower pore space connectivity and larger pools of mineral-associated organic matter (Schimel, 2021). Given observed differences in SOM composition (Text S5) and soil structure, we hypothesize that factors including oxygen availability and alternative electron acceptors may influence heterotrophic respiration to a greater degree than soil C as depth increases.

We also found a suite of correlations between elements and potential soil respiration that may reflect the influence of vegetation across rooting profiles; however, associations between inorganic nutrients (NH_4^+, NO_3^-, PO_4^{3-}) and respiration were conspicuously absent ($p>0.05$, Table S1) (Fan et al., 2022; Mori et al., 2018; Nicolás et al., 2019; Subedi et al., 2021). Mg, Mn, Zn, and sulfate were correlated to potential soil respiration and are known to have strong impacts on plant productivity that provides chemically labile C sources for microbial respiration (Chao et al., 2019; Gransee & Führs, 2013; Opfergelt et al., 2017). Mn can also influence soil respiration by regulating the activities of Mn peroxidase enzyme, a lignin-degrading enzyme produced by fungi and *Actinobacteria* (Kranabetter et al., 2021; Li et al., 2021; Neupane et al., 2023; Santos & Herndon, 2023; Whalen, 2017). Because total N corresponded to potential soil respiration, the lack of relationship between respiration and inorganic nutrients may indicate organic nutrients as key drivers of soil respiration. Alternatively, inorganic nutrient limitations that vary tremendously through space and time may not be observable across different ecosystems at the continental scale (Taylor & Townsend, 2010; M. Zhang et al., 2021).

In addition to patterns in soil physicochemistry, we observed geographic patterns in potential soil respiration that contrasted with some previous estimates (Nissan et al., 2023), including high rates of potential soil respiration in the midwestern and mid-Atlantic regions, and at high elevations (Figure S5). A notable difference between Nissan et al. and the current study is that Nissan et al. report simulated mean annual values of heterotrophic respiration in soils, while the current study reports the measured potential respiration rates of sieved soils collected during the summer months. Because high latitude and high elevation ecosystems can exhibit intense, short-lived peaks of biomass during summertime (Siles et al., 2017), soils collected during this period may have relatively extreme rates of potential soil respiration that are averaged out at the annual scale. Another interpretation for higher potential soil respiration at high elevation is that relative humidity typically increases with elevation and thus can stimulate higher microbial activities and SOM decomposition (Berryman et al., 2014). In contrast, comparatively low potential soil respiration recorded in the Southeastern United States could also reflect the comparatively low C content of these soils that has been associated with faster turnover rates and high year-round temperatures (Brye et al., 2016).

Text S5. SOM composition and relationship with potential soil respiration

Differences in SOM composition with soil depths and across the continental United States were associated with potential soil respiration, supporting previous studies showing relationships between SOM composition and soil respiration rates (Figure S5).(Bond-Lamberty & Thomson, 2010; Curiel Yuste et al., 2007; Changming Fang & John B Moncrieff, 2005). While patterns in SOM chemical across geographic regions were difficult to disentangle, the spatial distribution of NMF types suggested local similarity in

SOM composition in both layers (Figure S6-7), likely reflecting similar underlying chemistry, mineralogy, and/or biogeochemical processes (Brye et al., 2016).

For surface soils, NMF3 presented as the largest relative contributor to SOM composition in 20 soils across all biomes (i.e., highest weighting in H-matrix, hereafter, 'dominant signature', Figure S6). NMF2, NMF5, and NMF7 served as the dominant signature in at least 9 soils each. For subsoils, NMF5 and NMF2 were the dominant signature in 27 soils and 16 soils respectively distributed across all biomes in the continental United States (Figure S7). There was no single NMF*k* signature that could exclusively represent SOM composition of all sites in the same region for either surface or subsoils, suggesting that SOM composition at local sites is best summarized by a combination of multiple NMF*k*s.

The comparatively diverse SOM pools in surface soils contained more bioavailable compounds than subsoils, including protein-, amino sugar-, and lipid-like compounds (Figure S5(c)) (Jones, 1999; Marschner & Kalbitz, 2003). The number of formulae in these chemical classes declined with depth, and formula that were common to both soil layers primarily included chemical classes with low putative bioavailability such as lignin-, tannin-, and condensed hydrocarbon-like compounds (Marschner & Kalbitz, 2003).

There was a weak correlation between SOM composition and potential respiration in subsoils. NMF4 (associated with high-respiration soils) and NMF5 (associated with low-respiration soils) had the largest disparities in weighting across subsoils (Figure 2(e)). Consistent with observations from surface soils, subsoil NMF4 contained the largest proportion of amino sugar- and protein-like formula compared to other subsoil NMF*k*s, while NMF5 was almost entirely composed of lignin- and tannin-like compounds (Marschner & Kalbitz, 2003). The composition of water-extractable SOM in mineral subsoils is an emerging area of research, and it remains unclear how different SOM chemistries contribute to subsoil respiration (Rumpel & Kögel-Knabner, 2011). Our results suggest some consistencies in the chemical mechanisms of SOM bioavailability across soil horizons. However, one subsoil NMF*k* (NMF2) had unexpectedly large weightings in high respiration subsoils despite low bioavailability typically associated with its chemical constituents (Lehmann et al., 2020; Marschner & Kalbitz, 2003). The remaining subsoil NMF*k*s (1 and 3) were present in both low- and high-respiration subsoils. This denotes that factors beyond chemical recalcitrance or beyond the most commonly measured (water-extractable) SOM pool are critical to understanding belowground C cycling (Angst et al., 2021; H. Zhang et al., 2020).

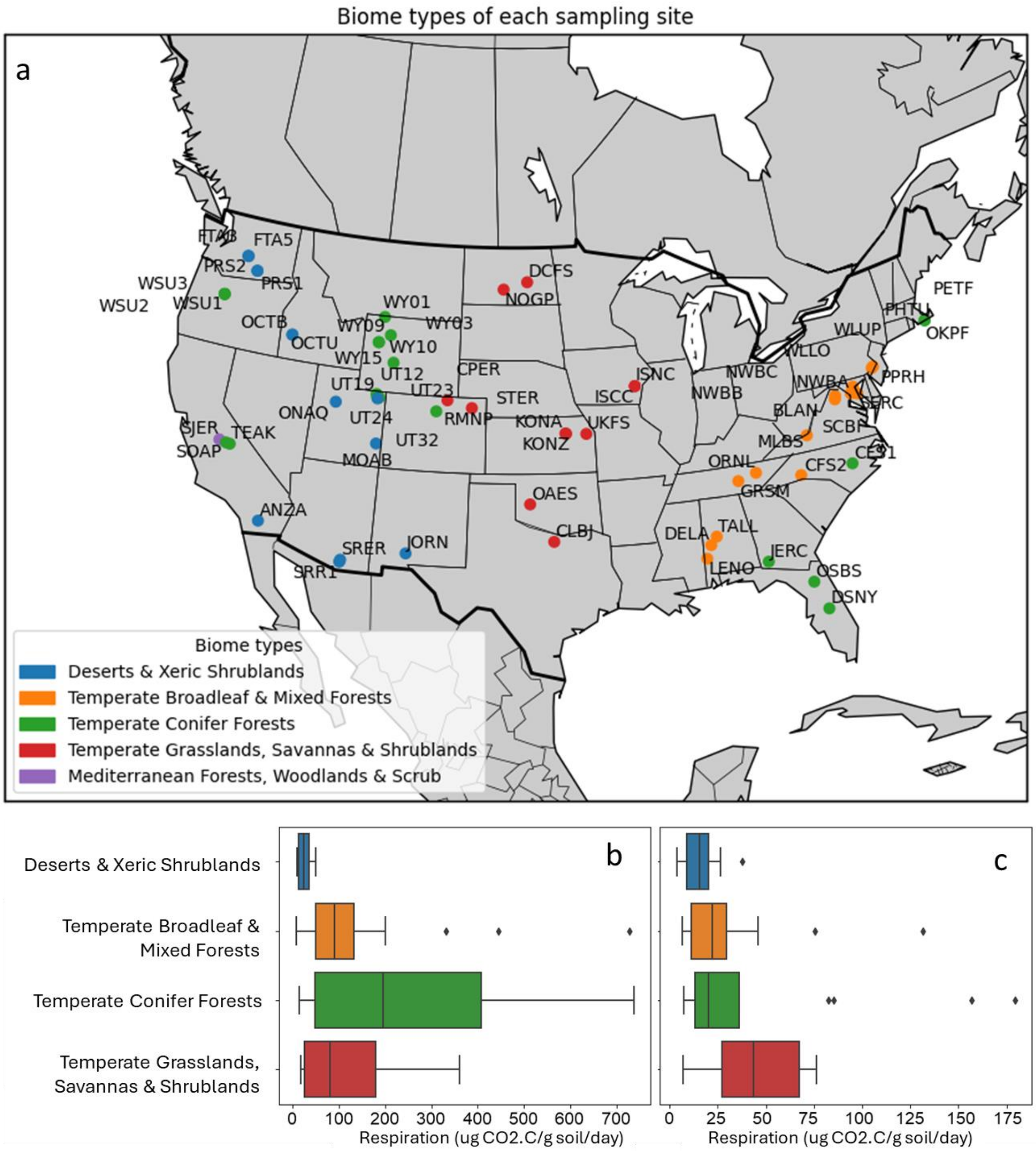

Figure S1. Sampling locations, sample names, and their biome types obtained from WWF terrestrial ecoregions (a). Potential soil respiration rates across biomes in b) surface and c) subsoil.

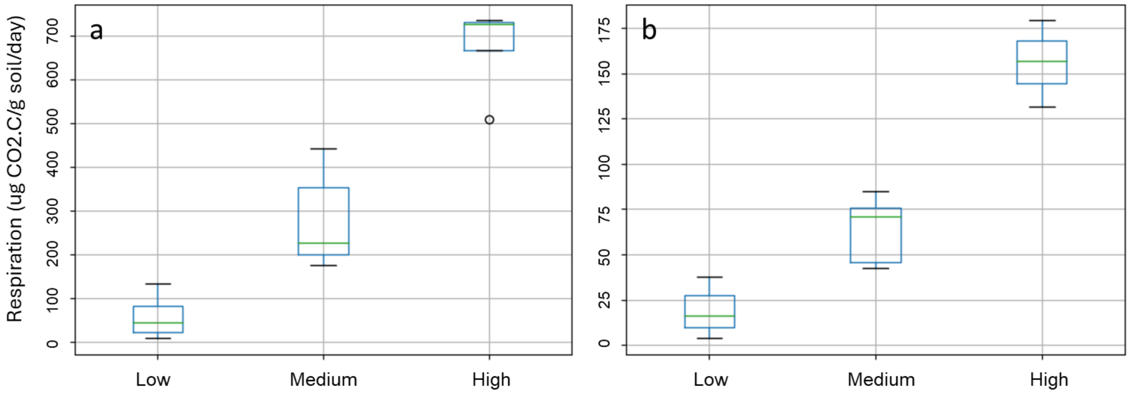

Figure S2. K-means clustering based grouping of potential soil respiration rates in a) surface soils and b) subsoils.

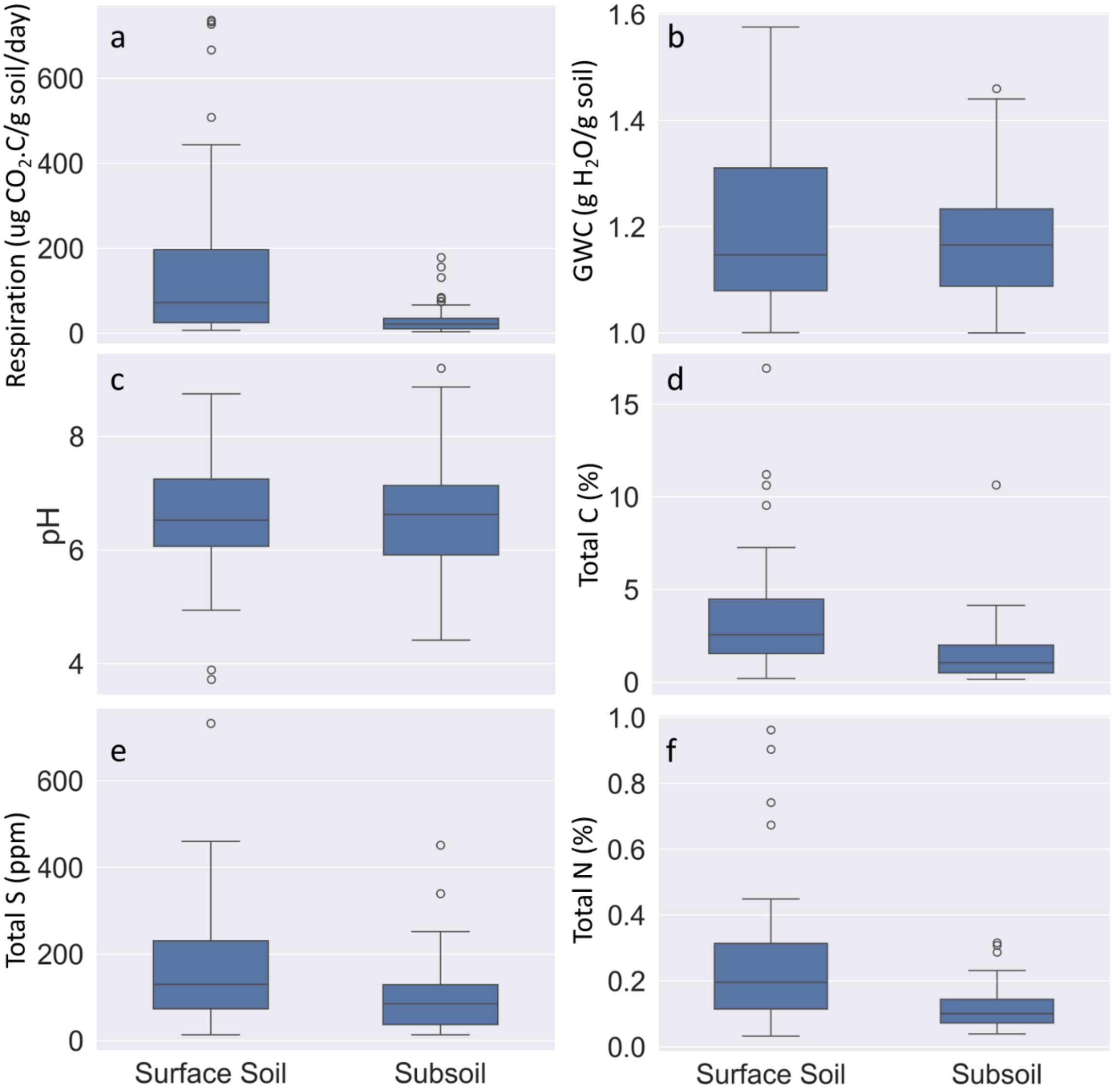

Figure S3. Boxplots of selected soil physicochemical variables between surface and subsoils. a) potential soil respiration, b) moisture content, c) pH, d) total C, e) total S, f) total N.

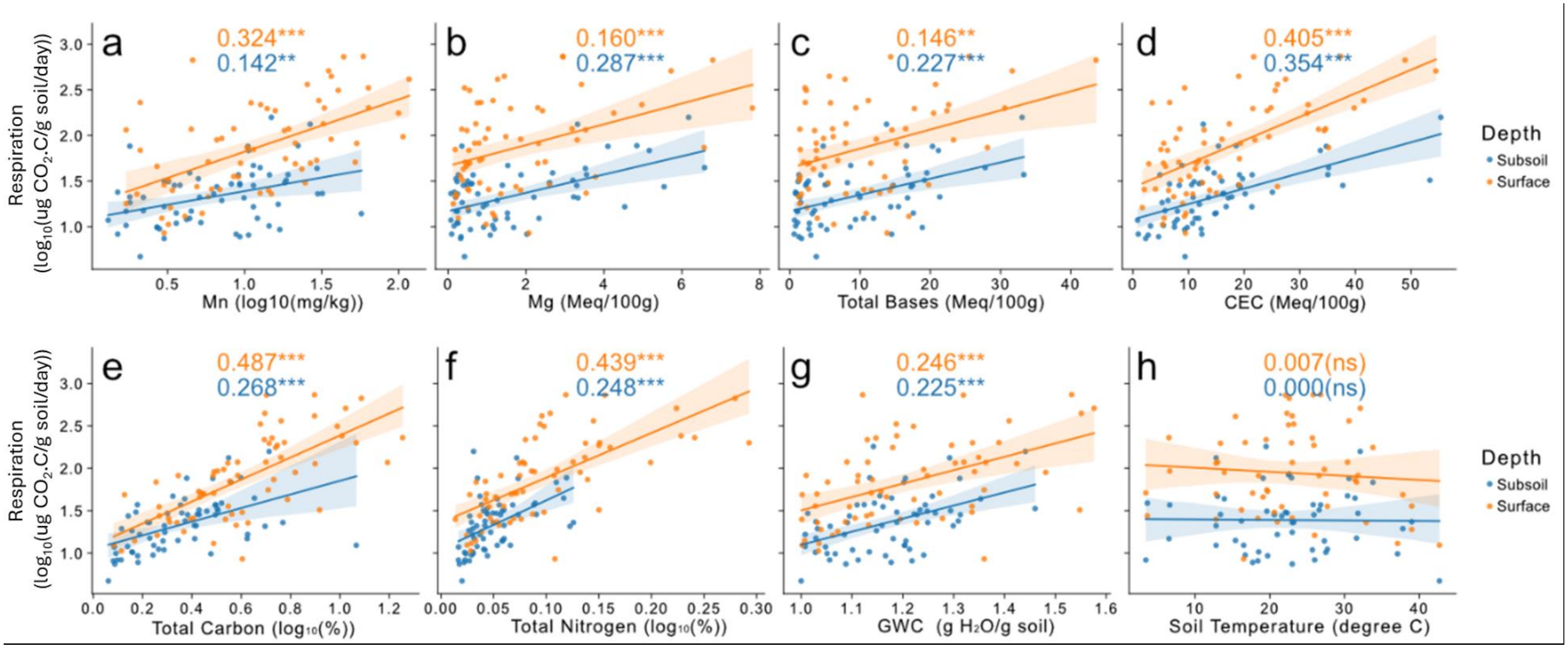

Figure S4. The relationship between soil characteristics and potential soil respiration. (a-h) show Manganese (Mn), Magnesium (Mg), Total Bases, CEC, Total C, Total N, GWC, and Soil Temperature, respectively. Orange represents surface soils and blue represents subsoils. Lines denote the fitted linear regression function. Numbers on each panel are R^2 value from linear regression, the stars behind represents statistical significance (*** ($p \leq 0.001$), **($p \leq 0.01$), ns ($p > 0.05$)).

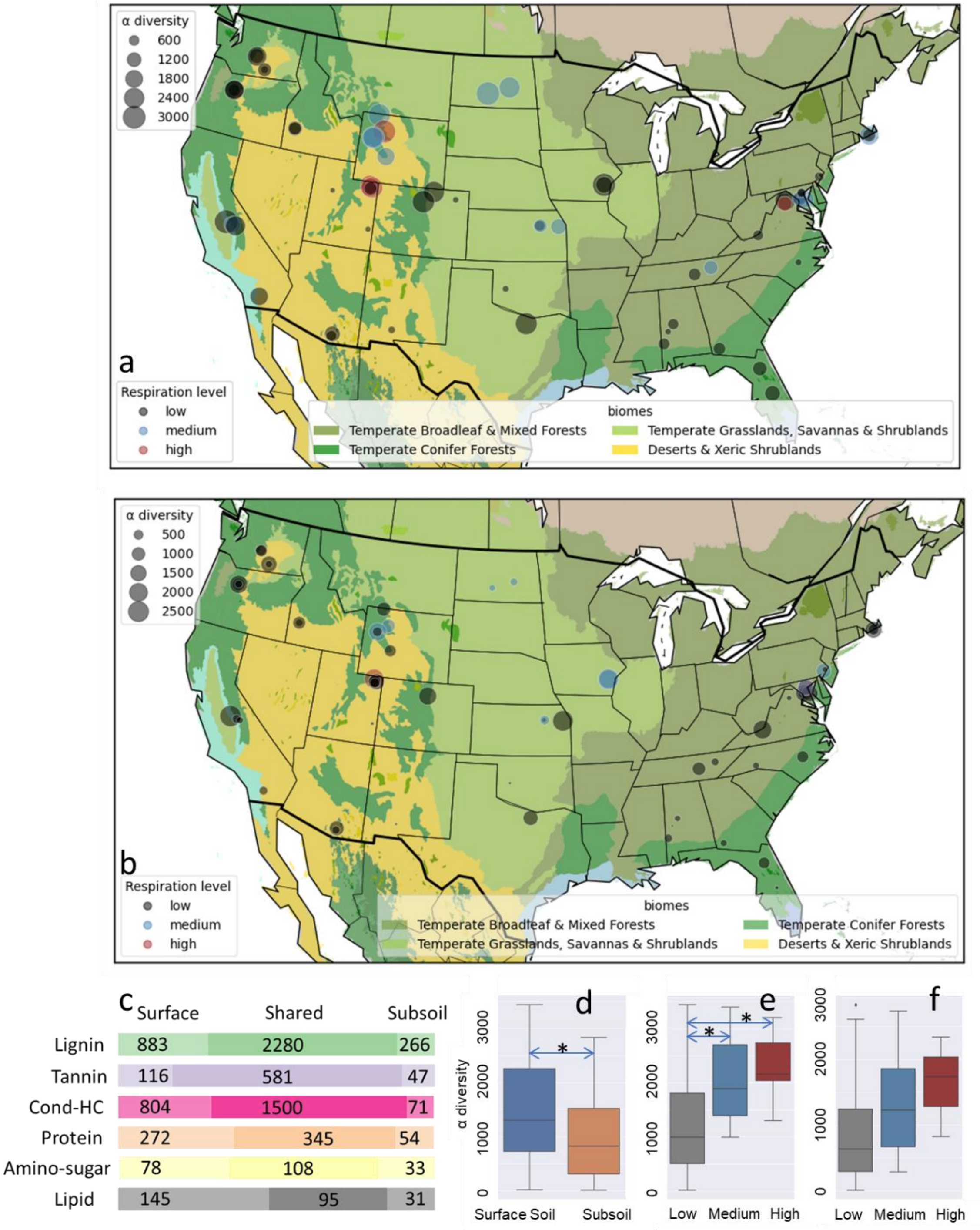

Figure S5. Spatial distribution of soil respiration levels (labeled by colors) and alpha diversity of SOM pools in each sample (bubble sizes) of a) surface soils and b) subsoils. Soil respiration levels are determined by k-means clustering on potential soil respiration rates (Figure S2). Soils from temperate conifer forests and temperate grasslands, savannas & shrublands have relatively higher respiration rates compared to other biomes (Figure S1). (c) The number of shared and unique SOM compounds identified between surface and subsoils, grouped by van Krevelen classification. (d) Alpha diversity of SOM in surface vs. subsoil soils ($p < 0.05$ from ANOVA, *:

$p<0.05$ from Tukey's HSD test). Alpha diversity of SOM across different levels of potential soil respiration in surface soils (e) and subsoils (f) ($p < 0.05$ from ANOVA, *: $p<0.05$ from Tukey's HSD test).

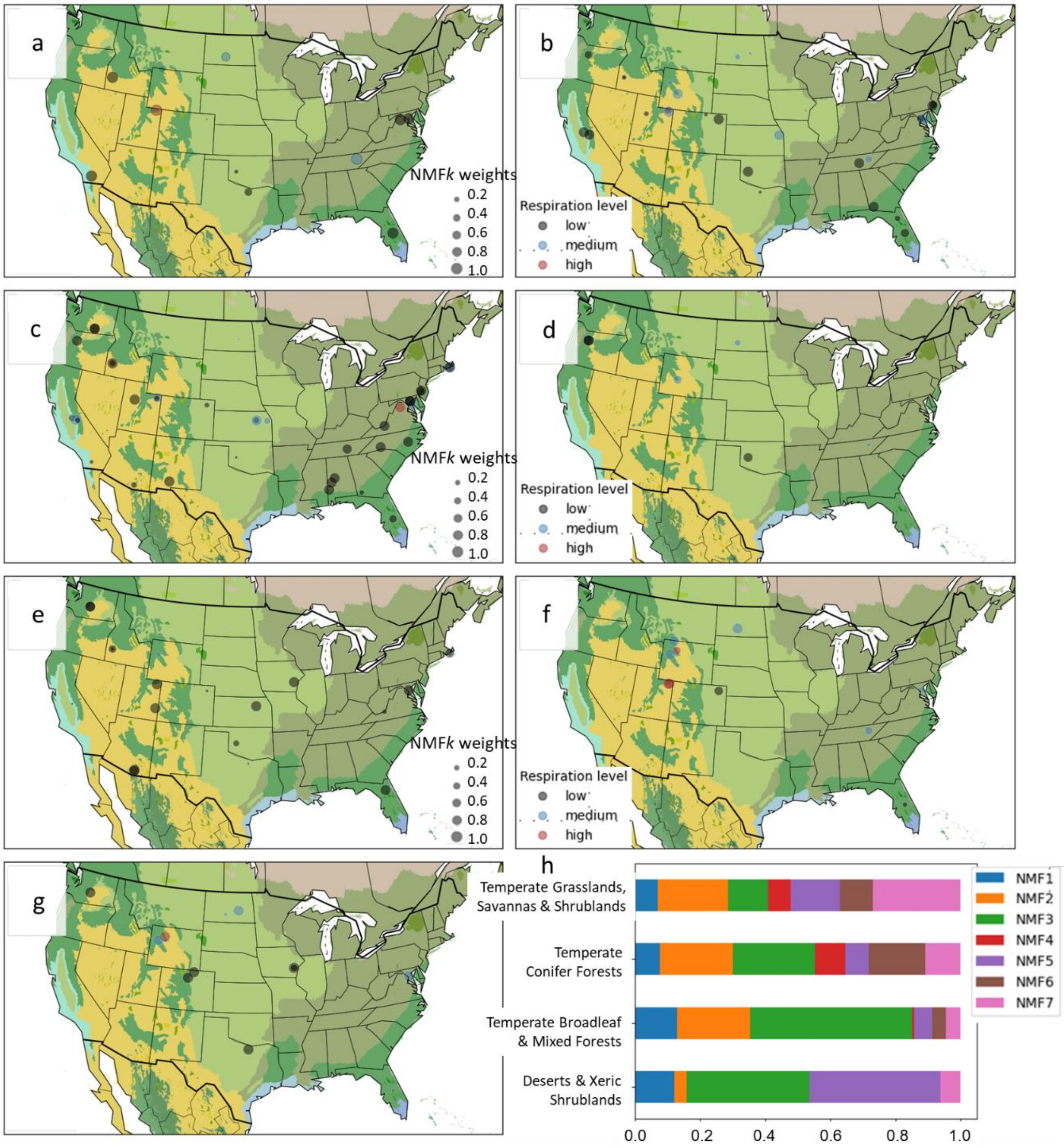

Figure S6. Normalized weights for each surface soil NKF*k* are shown sequentially in each map (a-g: NMF1-7). Weights are shown by bubble size, and bubbles are colored by respiration level. The relative contribution of the 7 types in each biome is shown by the stacked bar chart (h). Biomes and sample sizes are as follows: Deserts & Xeric Shrublands (N = 13), Temperate Broadleaf & Mixed Forests (N = 17), Temperate Conifer Forests (N = 21), Temperate Grasslands, Savannas & Shrublands (N = 11).

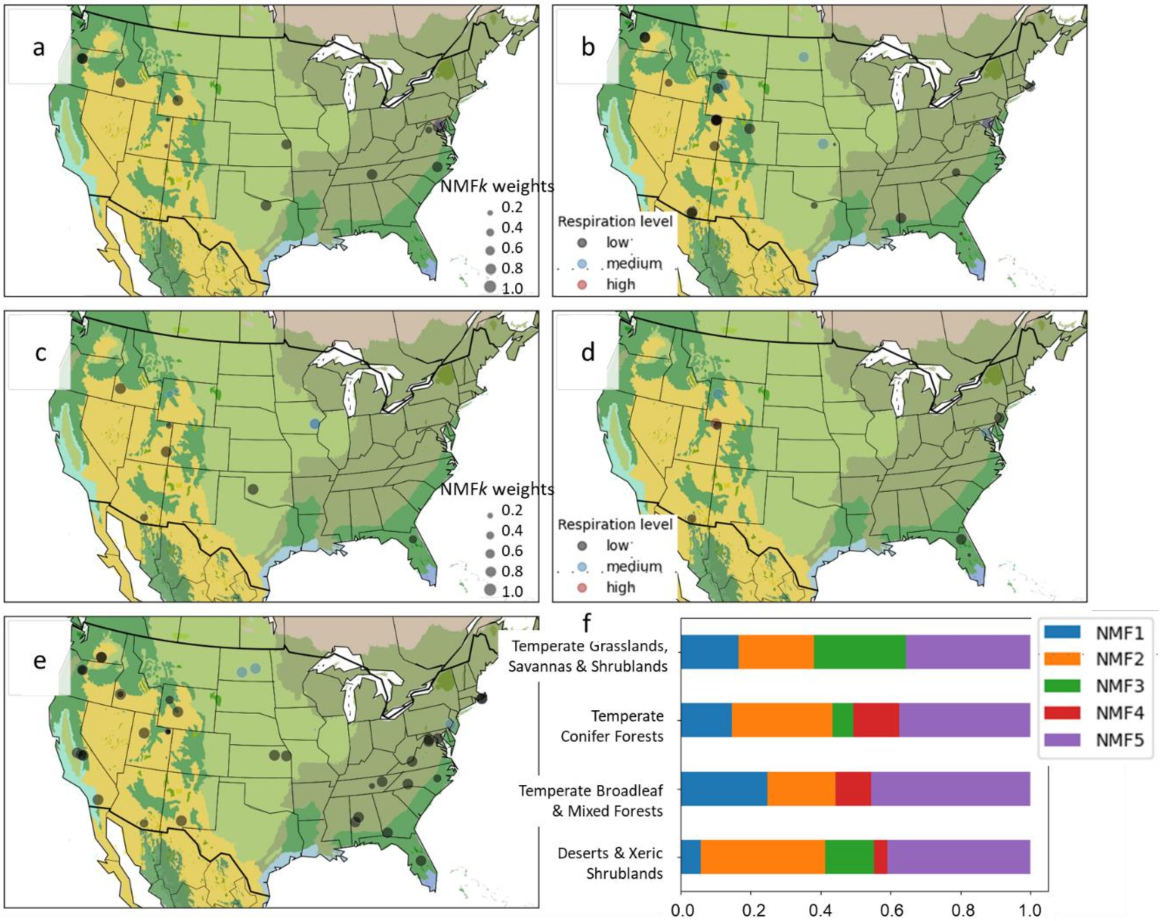

Figure S7. Normalized weights for each subsoil NKFk are shown sequentially in each map (a-e: NMF1-5) . Weights are shown by bubble size, and bubbles are colored by respiration level. The relative contribution of the 5 types in each biome is shown by the stacked bar chart (f). Biomes and sample sizes are as follows: Deserts & Xeric Shrublands (N = 13), Temperate Broadleaf & Mixed Forests (N = 17), Temperate Conifer Forests (N = 21), Temperate Grasslands, Savannas & Shrublands (N = 9).

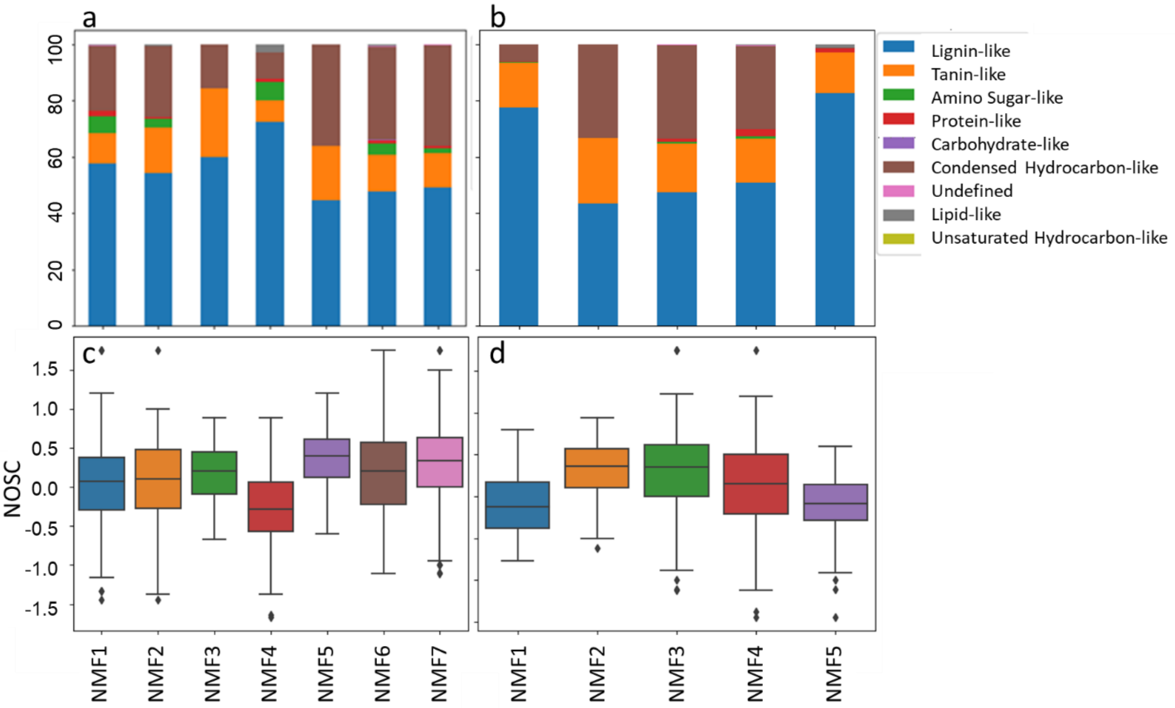

Figure S8. Relative contribution of each compound class to each NMF*k* in a) surface soil and b) subsoil. Boxplot shows the Nominal Oxidation State of Carbon (NOSC) for formula in each NMF*k* in c) surface soil and d) subsoil. Only formula with normalized weights of greater than 0.5 are included here.

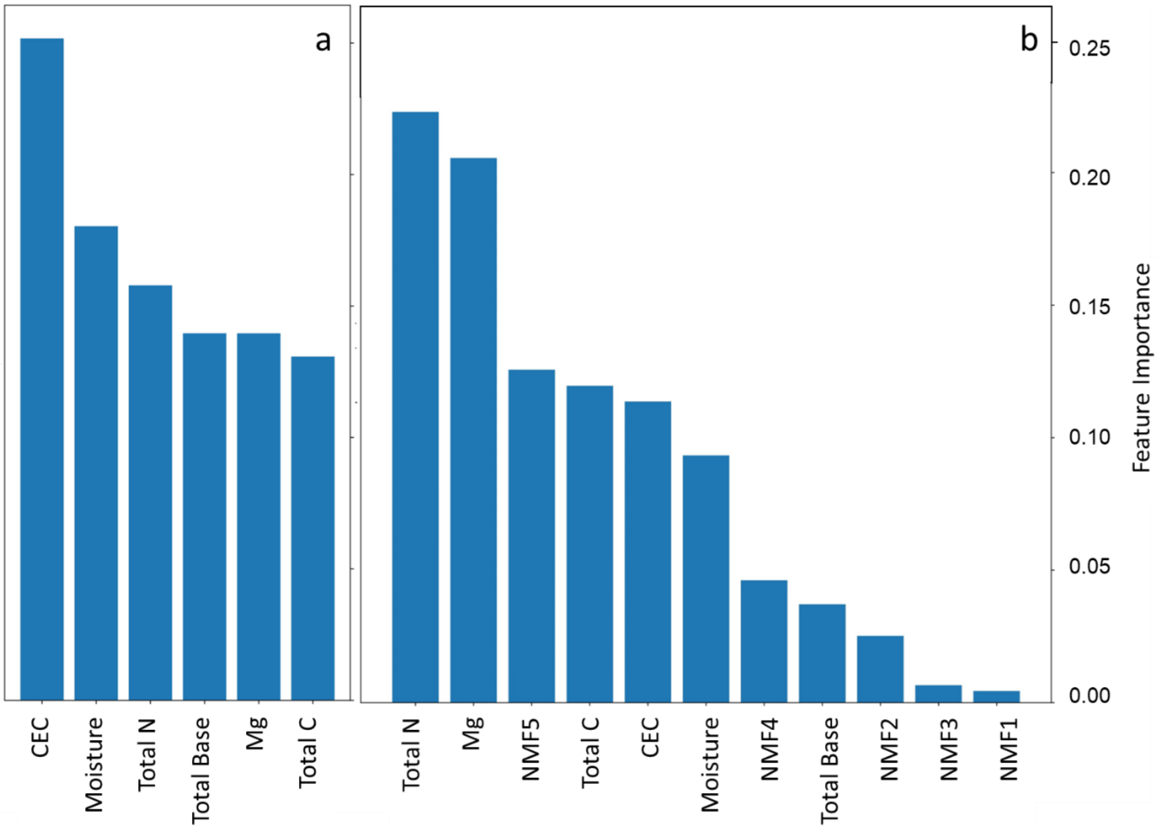

Figure S9. Relative importance of each predictor in subsoil potential respiration models. a) Physicochemistry Model, with physicochemical variables only. b) Physicochemistry & SOM model with both physicochemical variables and SOM composition. The model with SOM composition alone for subsoil did not yield adequate performance (Table 1) and therefore is not reported here.

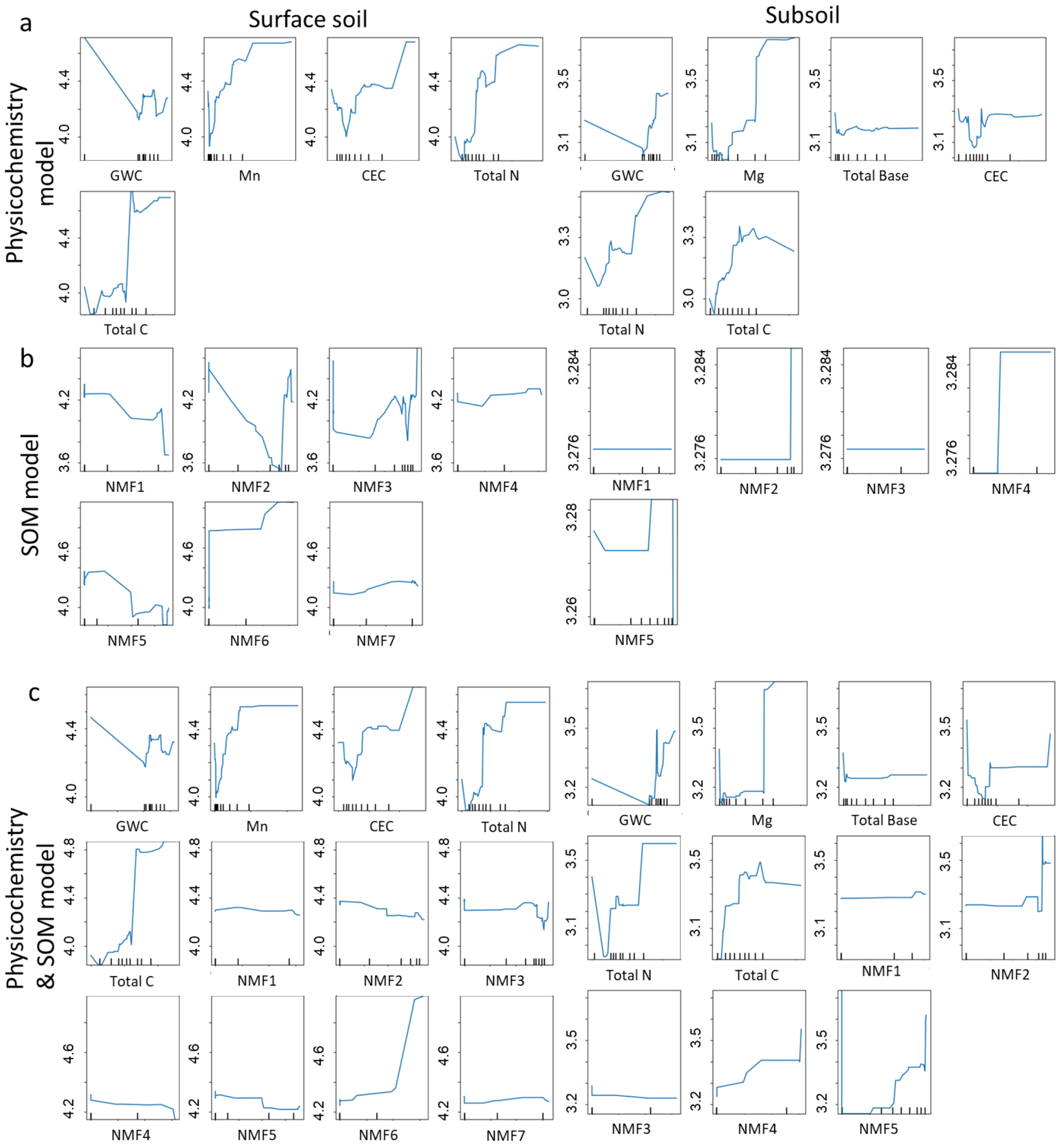

Figure S10. Partial dependence of potential soil respiration to soil physicochemistry and/or SOM composition in surface and subsoil models. a) Physicochemistry model with physicochemical variables for surface soil (left) and subsoil (right). b) SOM model with SOM composition for surface soil (left) and subsoil (right, low performance), c) Physicochemistry & SOM model with both physicochemical and SOM composition variables for surface soil (left) and subsoil (right).

	Surface R^2	Surface p-value	Subsoil R^2	Subsoil p-value
Mn	**0.324**	**0.000**	**0.142**	**0.003**
Mg	**0.160**	**0.001**	**0.287**	**0.000**
K	0.004	0.638	0.053	0.071
Na	0.005	0.577	0.026	0.211
B	**0.119**	**0.006**	0.018	0.295
Zn	**0.173**	**0.001**	**0.102**	**0.011**
Fe	**0.089**	**0.017**	0.043	0.106
Cu	**0.092**	**0.016**	**0.133**	**0.004**
Total Base	**0.146**	**0.002**	**0.227**	**0.000**
CEC	**0.405**	**0.000**	**0.354**	**0.000**
Total C	**0.487**	**0.000**	**0.268**	**0.000**
Total N	**0.439**	**0.000**	**0.248**	**0.000**
Total S	**0.080**	**0.028**	0.036	0.160
GWC	**0.246**	**0.000**	**0.225**	**0.000**
Soil T	0.007	0.545	0.000	0.919
pH	**0.116**	**0.004**	0.007	0.513
SO4	**0.172**	**0.001**	0.002	0.759
P	0.001	0.855	0.003	0.695
NH4	0.002	0.761	0.000	0.992
NO3	0.004	0.634	0.004	0.634
Sand%	**0.140**	**0.001**	**0.176**	**0.000**
Silt%	**0.081**	**0.017**	**0.077**	**0.022**
Clay%	**0.157**	**0.001**	**0.182**	**0.000**
Elevation	**0.136**	**0.006**	**0.090**	**0.029**
alpha_div	**0.159**	**0.001**	**0.143**	**0.003**

Table S1. Coefficient of Determination between potential soil respiration and soil physicochemistry (Pearson's correlation R-square). The bold texts highlight significant relationships with p-value <0.05.

	Physiochemistry Model	SOM Model	Physicochemistry & SOM Model
Surface_CV (RMSE)	0.80	1.05	0.82
Surface_test (RMSE)	0.98	0.89	0.82
Surface_test (R^2)	0.44	0.54	0.62
Subsoil_CV (RMSE)	0.60	0.82	0.67
Subsoil_test (RMSE)	0.46	0.80	0.49
Subsoil_test (R^2)	0.43	0.08	0.36

Table S2. Model performance for predictions of potential soil respiration with physicochemical variables (Physiochemistry Model), SOM by NMF*k* signatures (SOM Model), and combined physicochemical and SOM variables (Physiochemistry & SOM Model) for average 5-fold cross-validation accuracies (training soils, RMSE), and testing sample accuracies (RMSE, R^2).

Hyperparameter name	param_distributions	Physicochemistry Model		SOM Model		Physicochemistry & SOM Model	
		Surface	Subsoil	Surface	subsoil	surface	subsoil
n_estimators	randint(50,5000)	1213	1722	422	636	1392	351
max_depth	randint(2,60)	31	58	14	7	40	16
max_features	randint(1, X.shape[1])	1	6	2	5	3	7
min_samples_split	randint(2, 10)	6	6	4	6	7	9
learning_rate	[0.0001, 0.001, 0.01, 0.1, 1.0]	0.01	0.01	0.1	0.001	0.1	0.1
ccp_alpha	expon(scale=0.1)	9.42e-4	0.0173	0.0435	1.77e-3	1.86e-5	6.59e-4

Table S3. Hyperparameter tunning settings and the tuned hyperparameters used in each model.

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