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Two-dimensional NMR spectroscopy strongly enhances soil organic matter composition analysis

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Soil organic matter (SOM) is the largest terrestrial carbon pool and strongly affects soil properties. With climate change, understanding SOM processes and turnover and how they could be affected by increasing temperatures becomes critical. This is particularly key for organic soils as they represent a huge carbon pool in very sensitive ecosystems, like boreal ecosystems and peatlands. Nevertheless, characterization of SOM molecular composition, which is essential to elucidate soil carbon processes, is not easily achieved, and further advancements in that area are greatly needed. Solid-state one-dimensional (1D) 13C nuclear magnetic resonance (NMR) spectroscopy is often used to characterize its molecular composition, but only provides data on a few major functional groups, which regroup many different molecular fragments. For instance, in the carbohydrates region, signals of all monosaccharides present in many different polymers overlap. This overlap thwarts attempts to identify molecular moieties, resulting in insufficient information to characterize SOM composition.
Here we show that two-dimensional (2D) liquid-state 1H–13C NMR spectra provided much richer data on the composition of boreal plant litter and organic surface soil. The 2D spectra indeed resolved overlaps observed in 1D 13C spectra and displayed signals from hundreds of identifiable molecular groups. For example, in the aromatics region, signals from individual lignin units could be recognized. It was hence possible to follow the fate of specific structural moieties in soils. We observed differences between litter and soil samples, and were able to relate them to the decomposition of identifiable moieties. Sample preparation and data acquisition were both simple and fast.
Further, using multivariate data analysis, we aimed at linking the detailed chemical fingerprints of SOM to turnover rates in a soil incubation experiment. With the multivariate models, we were able to identify specific molecular moieties correlated to variability in the temperature response of organic matter decomposition, as assessed by Q10.
Thus, 2D NMR methods, and their combination with multivariate analysis, can greatly improve analysis of litter and SOM composition, thereby facilitating elucidation of their roles in biogeochemical and ecological processes that are so critical to foresee associated feedback mechanisms on SOM turnover as a result of global environmental change.