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Spectral fingerprinting of soil organic matter composition

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The determination of soil organic matter (SOM) composition relies on a variety of chemical and physical methods, most of them time consuming and expensive. Hitherto, such methodological limitations have hampered the use of detailed SOM composition in process-based models of SOM dynamics, which usually include only three poorly defined carbon pools. Here we show a novel approach merging both near and mid infrared spectroscopy into a single fingerprint for an expeditious prediction of the molecular composition of organic materials in soil, as inferred from a molecular mixing model (MMM) based on 13C nuclear magnetic resonance (NMR), which describes SOM as a mixture of common biologically derived polymers. Infrared and solid-state 13C NMR spectroscopic measurements were performed on a set of mineral and organic soil samples presenting a wide range of organic carbon content (2 to 500 g kg-1), collected in a boreal heathland (Storgama, Norway). The implementation of the MMM using 13C NMR spectra allowed the calculation of five main biochemical components (carbohydrate, protein, lignin, lipids and black carbon) for each sample. Partial least squares regression models were developed for the five biopolymers using outer product analysis of near and mid infrared spectra (Infrared-OPA). All models reached ratios of performance to deviation (RPD) above 2 and specific infrared wavenumbers associated to each biochemical component were identified. Our results demonstrate that Infrared-OPA provides a robust and cost-effective fingerprint of SOM composition that could be useful for the routine assessment of soil carbon pools.