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Molecular characterisation of soil organic matter by laser-desorption ionization Fourier-transform ion cyclotron resonance mass spectrometry (LDI-FT-ICR-MS)

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Soil organic matter (SOM) characterisation has been an analytical challenge for decades. On one hand, methods like humic substances extraction describe large pools of molecules, but these extractions target operationnally- rather than chemically-defined pools. On the other hand, specific compound analysis provides a more precise overview on the molecules present in the soil, but the sum of these molecules represents only a minor portion of the soil organic matter. Despite these shortcomings, soil organic matter characterisation is used in many concepts of soil science. For example, the soil aggregation hierarchical model describes the physical organisation of soils into fractions bound together by organic matter of different quality for each size fraction. Due to the method inadequation, most of these concepts still need to be validated.
We took advantage of a unique analytical set-up coupling laser-desorption ionization (LDI) to ultrahigh-resolution mass spectrometry via the Fourier-transform ion cyclotron resonance technique (FT-ICR-MS) to further characterise soil organic matter and to validate the soil aggregation hierarchical model. Soil aggregates (3-5 mm) were collected from two soils, a cambisol (32 % clay, 4.2 %C), and a loess-derived soil (15% clay, 1.6 %C). Aggregates were fractionated by fast wetting into <63, 63-125, 125-250 and > 250 μm fractions. These fractions were air-dried and ground to powder prior to analysis. LDI-FT-ICR-MS analyses were performed on otherwise untreated samples. Thousands of molecular formulae were identified in each samples, many of them could be associated with polyphenolic structures. The combination of LDI with ultrahigh-resolution FT-ICR-MS offers fundmentally new insights into soil organic matter, one of the largest organic matter pools on Earth.