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Non-target screening of soil and litter derived dissolved organic matter using high resolution mass spectrometry (LC-QTOF-MS)

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Non-target screening using high resolution LC-QTOF-MS (Liquid Chromatography - Quadrupole Time-of-flight Mass Spectrometry) is often used e.g. to screen for emerging contaminants in surface water chemistry research. However, in the field of soil science, it is still a relatively new approach. LC-QTOF-MS could facilitate research on the chemical interactions between molecules in important soil processes as podzolization and organic matter (OM) stabilization. We developed a non-target screening method using high-resolution LC-QTOF-MS/MS for the characterization of dissolved organic matter (DOM) extracted from soil and (forest floor) litter material. The MS/MS mode of LC-QTOF facilitates the retrieval of molecular fragment data, that can be utilized to improve the structural characterization of OM. Large parts of our LC-QTOF-MS workflow can be automated, which is essential when investigating the numerous chemicals present in bulk SOM.

The method we developed can be divided into two parts; (1) measuring DOM samples (extracted from soil and plant litter material) with LC-QTOF-MS (and/or MS/MS), and (2) semi-automated data analysis. Samples were separated with ultra-high performance liquid chromatography (UHPLC) and eluting compounds were ionized by electrospray ionization (ESI) operating in negative (-) mode. The resulting data was processed (part two) with in-house developed software based on R which harmonizes various open source and vendor data processing tools (e.g. OpenMS, GenForm and Bruker DataAnalysis). Our workflow consists of (a) data pre-treatment (e.g. automatic recalibration and data export to mzML), (b) extraction and alignment of chromatographic and mass spectral data, (c) rule based filtering based on minimal intensity, absence in sample blanks and ubiquitous presence in replicates and (d) automatic calculation of molecular formulae based on high resolution MS and MS/MS data. Candidate formulas that did not fulfil basic chemical criteria were removed. First tests using samples from soil and plant litter derived DOM yielded information on the dominant molecular compound classes (e.g. lignin and lipids), indicating that differences in DOM molecular composition were larger between plant litter and soil derived DOM from one location then among similar DOM sources from different locations. By using LC and MS/MS, our method represents an alternative way to open the SOM ‘black box’ and turn it into a ‘grey box’ and expands the possibilities for OM characterization from often used techniques such as NMR spectroscopy and pyrolysis gas chromatography mass spectrometry (pyr-GC-MS).