



Identifying metabolites related to nitrogen mineralisation using ^1H NMR spectroscopy

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Exploring new analysis techniques to enhance our knowledge of the various metabolites within our soil systems is imperative. Principally, this knowledge would allow us to link key metabolites with functional influences on critical nutrient processes, such as the nitrogen (N) mineralisation in soils. Currently there are few studies that utilize proton nuclear magnetic resonance spectroscopy (^1H NMR) to characterize multiple metabolites within a soil sample. The aim of this research study was to examine the effectiveness of ^1H NMR for isolating multiple metabolites that are related to the mineralizable N (MN) capacity across a range of 35 Irish grassland soils. Soils were measured for MN using the standard seven day anaerobic incubation (AI-7). Additionally, soils were also analysed for a range of physio-chemical properties [e.g. total N, total C, mineral N, texture and soil organic matter (SOM)]. Proton NMR analysis was carried on these soils by extracting with 40% methanol:water, lyophilizing and reconstituting in deuterium oxide and recording the NMR spectra on a 400MHz Bruker AVANCE III spectrometer. Once the NMR data were spectrally processed and analysed using multivariate statistical analysis, seven metabolites were identified as having significant relationships with MN (glucose, trimethylamine, glutamic acid, serine, aspartic acid, 4-aminohippuric acid and citric acid). Following quantification, glucose was shown to explain the largest percentage variability in MN (72%). These outcomes suggest that sources of labile carbon are essential in regulating N mineralisation and the capacity of plant available N derived from SOM-N pools in these soils. Although, smaller in concentration, the amino acids; 4-aminohippuric acid, glutamic acid and serine also significantly ($P < 0.05$) explained 43%, 27% and 19% of the variability in MN, respectively. This novel study highlights the effectiveness of using ^1H NMR as a practical approach to profile multiple metabolites in soils simultaneously, and increasing the potential to identify those related to various soil processes.