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Molecular investigations of the nature, occurrence and behaviour of phytic acid in soils using ion chromatography and high-resolution mass spectrometry.

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Cycling of phosphorus (P) in the environment plays a fundamental role in agricultural production and the health of soil and freshwater ecosystems. However, the contribution of organic phosphorus (Po) species to biological processes is not fully understood. Characterisation of Po for soil analysis is based on operational definitions of chemically extracted "pools" of P. While this approach is sufficient for studying bulk chemistry processes, it provides limited insights into the molecular mechanisms of organic phosphorus in the environment.

Attempts to characterise soil Po in more detail have mostly focused on the use of 31P nuclear magnetic resonance (NMR) spectroscopy. NMR can identify classes of Po compounds, for example phosphate monoesters, or diesters. However, potentially many tens or hundreds of compounds can contribute to a given signal in an NMR spectrum, since individual molecular species of Po cannot be resolved using this approach. In contrast, high resolution mass spectrometry (HRMS) has become a powerful tool in the analysis of complex biological samples and is being widely used in the field of metabolomics for the identification of significant compounds. HRMS can simultaneously resolve thousands of ions in a mass spectrum with the capability being extended still further by combination with chromatography such as ion chromatography (IC) to provide enhanced characterisations and quantitative determinations.

Phytic acid (IP6) is an important organic P compound, comprising up to 50 % of Po in soils. This paper presents results from the development and application of electrospray (ESI) HRMS and IC/HRMS techniques to the determination of IP6. ESI-HRMS is used to unequivocally identify the compound extracted from a soil matrix. IC quantification is found to be more rapid and sensitive than current 31P NMR techniques. The extraction efficiency of IP6 from a range of soils is determined and correlated with soil characteristics, such as organic and metal content. The degradation of IP6 from poultry litter is investigated, revealing dynamic potential for extraction of the compound, whereby soil microbial activity is required to breakdown the poultry litter matrix before degradation can take place. We demonstrate how molecular characterisation of IP6 using the latest analytical methods enables the study of the molecular level processes involving Po in the environment to better understand the role Po plays in the P cycle.