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# Characterisation of riverine dissolved organic matter using a hierarchy of mass spectrometric methods.

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The flux of dissolved organic matter (DOM) into rivers is rising due to a range of factors. These include both inputs of organic wastes from livestock production and the discharge of sewage effluent in lowland catchments, as well as the mobilisation of soil organic matter stores in response to climate change, land use change and the biogeochemical response to reduction in acid deposition in upland and boreal catchments. This trend is set to continue due to our changing climate and increasing population, meaning extra pressure is being exerted on ecosystems. There is a growing body of research showing that many DOM compounds are bioavailable and can be rapidly assimilated by stream biota, which may have important implications for nutrient cycling and riverine health. With this in mind, it is vital to gain a more comprehensive understanding of the composition of riverine DOM at a molecular level.

DOM is an extremely complex mixture of individual compounds and therefore poses some analytical challenges. Most often, DOM is quantified as a bulk nutrient fraction then characterised by parameters such as hydrophobicity, molecular weight, aromaticity and functional group. However, recent advancements in analytical approaches can help allowing more detailed characterisation to compound level. Typically, molecular-scale analysis of DOM has been carried out in a targeted way, where compounds of interest are analysed. However, when the aim is to characterise the range of compounds comprising the DOM pool a more untargeted approach is necessary. Therefore, here, we propose a hierarchical approach to DOM characterisation using a suite of cutting-edge analytical techniques in order to obtain a wide analytical window spanning different size fractions and polarities. We use extractions followed by a combination of gas chromatography-mass spectrometry (GC-MS) and GC-quadropole-time-of-flight-MS (GC-Q-TOS-MS) to characterise the non-polar and polar ‘building block’ (i.e. amino acid/carbohydrate) fractions. The polar, intermediate molecular weight fraction is analysed using direct-infusion high-resolution MS (DI-MS) and the macromolecular material (e.g. lignin) is identified using pyrolysis coupled with GC/MS.

Here we present a number of UK-based case studies to illustrate the power of using this combination of analytical techniques to provide a truly untargeted approach to DOM characterisation. The results show that this approach allows determination of the differences between the molecular composition of waters depending on their catchment character, land use and management. This detailed information is now being used to aid DOM source appointment within catchments, which is key for managing water quality. These data are also allowing the identification of compounds of interest for further study with regards to biotic response to in-stream DOM.