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Exploring dissolved organic matter (DOM) signatures across contrasting UK landscapes using a high-resolution mass spectrometry 'fingerprinting' approach.

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Dissolved organic matter (DOM) plays a vital role in river ecosystem function and therefore understanding its composition is key. DOM has important implications for nutrient cycling and riverine health and with this in mind, it is vital to gain a more comprehensive understanding of the composition of riverine DOM at a molecular level and how this varies across contrasting landscapes. There are many factors which will influence DOM signatures, from differences in climate, soil type/geology, land-use, as well as intensity and nature of anthropogenic activity. Through understanding the potential relationships between these factors and DOM composition, we can gain key information regarding both sources of riverine DOM within river catchments, aiding pollution mitigation strategies, and how signatures may vary under changing climate and/or land-use.

The analysis of DOM poses a significant analytical challenge due to its complexity, however the advances in mass spectrometry now allows detailed characterisation at molecular scale. This study examines the DOM composition across 56 UK field sites spanning contrasting landscapes, including four different geologies/soil types. Additionally, 18 effluents from UK sewage treatment works (STW) were investigated. River water samples were collected and an untargeted analysis carried out using direct-infusion high-resolution mass spectrometry (DI-MS) and the resultant DOM signatures across the samples were compared.

Principal component analysis (PCA) and hierarchical clustering analysis methodologies were applied and showed that the DOM molecular composition between sites could be distinguished according to landscape character. Specifically, the PCA analysis showed that contrasting geologies/soil types were separated by the derived Principle Component (PC) 2 while PC1

separated the riverine samples from the STW effluents in the analytical space. Explanatory variables including landcover, land-use and population density alongside bulk nutrient data were used to begin to elucidate the driving factors behind the PCs. In addition to differences in DOM signatures, further analysis of the molecular compositions identified anthropogenically derived organic compounds, for example, series of polypropylene glycol (PPG) and polyethylene glycol (PEG) oligomers, which were present in almost all landscapes across the UK, illustrating that they are now ubiquitous across riverine environments. Using these data, we can begin to provide generalisable information regarding the molecular composition of DOM across different UK landscapes.