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Concealed by darkness: combination of NMR and FT-ICR MS reveal the heterogeneous molecular natures of dissolved organic matter in fractured-rock groundwater from an unconfined aquifer.

MAXIME CYRIL BRIDOUX[1], GABRIEL GAIFFE[1], SÉBASTIEN SCHRAMM[2], PIERRE PACHOLSKI[2], GIOVANNI VINCI[3], SILVANA CANGEMI[3] AND RICCARDO SPACCINI[3]

[1]CEA
[2]Université de Lorraine
[3]Università di Napoli Federico II
Presenting Author: maxime.bridoux@cea.fr

Groundwater contained in aquifers are the largest reservoirs of liquid freshwater on earth and play an essential role in global water and carbon cycles. Groundwater contains an important pool of terrestrial organic carbon in the form a very complex mixture of dissolved organic compounds containing mainly C, H, O, N and S that represent a critical component of groundwater quality. The conventional view of how dissolved organic matter (DOM) behaves in groundwater suggests that it becomes less able to support biological activity over time [1]. However, recent research has found that a significant amount of organic carbon (13 Tg annually) released into surface waters through groundwater discharge appears to be quite biodegradable, challenging this traditional paradigm [2]. The unconfined Chalk aquifer is a crucial aquifer in Northern Europe, given its extensive usage for human purposes, with a significant portion reserved for drinking water. In France, the Chalk aquifer extends over approximately 20% of the metropolitan territory and supplies roughly 12 billion cubic meters of water annually, representing 70% of the drinking water utilized in the Northern region of the country.

In this study, we used NMR spectroscopy along with full scan ultrahigh resolution FT-ICR MS and high resolution Orbitrap tandem MS (MS/MS) to examine the molecular composition of DOM in fractured-rock groundwater and surface river water in two different watersheds in the unconfined chalk aquifer of Champagne, France. We utilized both ESI (-) and APPI(+) ionization techniques for the first time in aquifers to target both polar and non-polar compounds in groundwater and surface river DOM. Finally, we used ab-initio mass difference transformation networks (MDiNs) to visualize and investigate the biogeochemical relationships hidden in the full scan FT ICR-MS DOM spectra, providing critical new information about its chemical diversity and the set of microbial and abiotic reactions or pathways that produced it.

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