Profiling of groundwater dissolved organic matter by high resolution NMR spectroscopy

Y. LI[1], V. ROTH[1], N. HERTKORN[2], G. GLEIXNER[1*]

[1]Max Planck Institute for Biogeochemistry Jena, Postbox 100164, 07701 Jena, Germany

[2]Helmholtz Zentrum Muenchen, German Research Center for Environmental Health, Analytical BioGeoChemistry, 85764 Neuherberg, Germany

[*]correspondence: gerd.gleixner@bgc-jena.mpg.de

While karst landscapes provide ~25% of the world's population with drinking water [1], comprehensive understanding of respective aquifer structure and groundwater chemistry remains limited even if substantial transformation of organic matter has been reported [2]. In our study, chemical structures of groundwater dissolved organic matter (DOM) dependent on land use, hydrochemistry and geological structures have been investigated.

Differences in carbon and proton chemical environments in groundwater DOM from Hainich critical zone (Northwestern Thuringia, Central Germany) were evaluated by high resolution NMR spectroscopy. Groundwater DOM obtained from agriculturally-used lower hillslopes (H5-1, H5-2 and H5-3) was quite different from that obtained from the higher hillslopes [3]. These DOM contained more numerous superimposed small NMR resonances in the aromatic region indicative of biogeochemical molecules, like polycarboxylic acids. Groundwater DOM from anoxic well H5-3 was distinct from that of oxic wells H5-1 and H5-2 and showed limited divergence of aliphatics, but smaller proportions of aromatics and olefins. Moreover, numerous superimposed small NMR resonances in the aromatic region were observed in H5-3 and those resonances could be further assigned to different, possibly polycyclic, polycarboxylic acids and oxygenated aromatics.

Moreover, the NMR results were in consistence with targeted metabolomic profiling of groundwater DOM based on mass spectrometry.

[1] Ford and Williams, Karst Hydrology and Geomorphology, *Wiley: Chichester. 561*, ***2007***. [2] Einsiedl *et al* (2007) *Geochimica et Cosmochimica Acta* **71**, 5474-5482. [3] Kohlhepp *et al* (2016) *Hydrology and Earth Sysrem Sciences.* doi:10.5194/hess-2016-374.