Application of neutral loss tandem MS and time-of-flight MS to identify anthropogenic compounds in fulvic acids

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The interactions of contaminants with dissolved organic matter (DOM) highly determines their transport, fate, and bioavailability in the aquatic environment. The main part of DOM in water can be attributed to fulvic acids (FA) and humic acids (HA) on an operationally-defined basis. Contaminants associated with or behaving like humic substances are a concern for groundwater because they are highly mobile and may not be completely removed during drinking water treatment. Furthermore those contaminants can be transformed by oxidation or disinfection steps to form further products of toxicological importance.

Beside for highly selective and sensitive analysis tandem mass spectrometry can be used for non-target screening to get a more comprehensive picture of a sample. For that purpose neutral loss scans can be used to reveal compounds with common structural moieties, e.g. acidic functional groups.

The objective of the presented work is to characterize FA fractions with respect to their anthropogenic contributions in isolated material from both a contaminated groundwater and a natural surface water [1, 2]. Neutral loss screening at the mass losses 44 (CO_2) and 116 (C_2H_4 $(CO_2)_2$) revealed aromatic and heterocyclic acids and succinic acids, predominantly in the contaminated sample. The further identification of the compounds was based on a combination of the sum formulae from accurate mass measurements with a Q-TOF instrument, information on the original contamination and the prevailing degradation processes in the aquifer [3]. Predominantly the FA fraction from the contaminated groundwater shows a considerable 'anthropogenic' content which has implications for its use for drinking water treatment.

[1] Zwiener *et al*. (1999) *Acta Hydrochim. Hydrobiol*. **27**, 208–213. [2] Kumke *et al*. (1999) *Acta Hydrochim.Hhydrobiol*. **27**, 409–415. [3] Ohlenbusch *et al*. (2002) *J. Chromatogr. A* **967**, 201–208.