



## **Analytical Determination of $K_{DOC}$ -Values of Polycyclic Musk Compounds with HS-SPME and GC/MS/MS**

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Polycyclic musk compounds, used as fragrances in cosmetics and detergents, get into rivers via domestic wastewater and sewage treatment plants and with sewage sludge as fertilizer into soils. Because of their persistence and lipophilic character they accumulate in biota, so they are pollutants with environmental relevance.

The coefficient  $K_{DOC}$  is used to quantify the distribution of substances between aqueous phase and dissolved organic matter (DOM) which is quantified by the determination of dissolved organic carbon (DOC). DOM is of specific relevance for the transport and fate of persistent and lipophilic compounds in the environment. The affinity to DOM increases, the more lipophilic a substance is. So the environmental mobility is enhanced with increasing binding on DOM. For that reason, measured  $K_{DOC}$ -values are important to predict the fate and behaviour of chemicals in the environment and should be used for environmental fate modelling purposes. LITZ ET AL. (2007) state that, to carry out a risk-assessment for polycyclic musk compounds, further research on their sorption-behaviour is necessary.

For the determination of  $K_{DOC}$ -values, different concentrations of humic acid were spiked with a multi-component stock solution. The samples were analysed with headspace solid-phase microextraction in combination with gas chromatography coupled with mass spectrometry (HS-SPME GC/MS/MS). The  $K_{DOC}$ -values were calculated according to YABUTA ET AL. (2004).

The method was validated with single substance stock solutions and with polycyclic aromatic hydrocarbons (PAHs). The results show that the method is applicable, repeatable and suitable to get  $K_{DOC}$ -values for many substances very fast, cheap and solvent-free.

With our results  $K_{DOC}$ -values for polycyclic musk compounds were determined for the first time.

### **Literature**

LITZ, N. TH., MÜLLER, J. AND BÖHMER, W. (2007): Occurrence of Polycyclic Musks in Sewage Sludge and their Behaviour in Soils and Plants. Part 2: Investigation of Polycyclic Musks in Soils and Plants. *J Soils Sediments* 7: 36-44

YABUTA, H., FUKUSHIMA, M., TANAKA, F., ICHIKAWA, H. AND TATSUMI, K. (2004): Solid-phase Microextraction for the Evaluation of Partition Coefficients of a Chlorinated Dioxin and Hexachlorobenzene into Humic Substances. *Anal. Sci.* 20: 787-791