Bibliographic Description

Combination of GC-MS and Chemometrics for the

Analysis of Compounds in Complex Environmental Samples

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Gas chromatography coupled with mass selective detection (GC-MS) is one of the most powerful hyphenated techniques for the analysis of complex environmental samples. The steady increase in new chemicals released to the environment demands new and improved analytical methods for the identification of ecotoxicologically relevant compounds. Therefore, new chemometric methods for GC-MS data evaluation will be presented in this work. These methods of qualitative GC-MS analysis were developed, validated and applied using environmental samples.

Experimental data was obtained from sediment extracts and polluted river water. Dialysates from semipermeable membrane devices (SPMDs), deployed in the strongly polluted Spittelwasser Creek (near Bitterfeld), were fractionated by flash chromatography. This simple pre-fractionation procedure allowed a fast GC-MS screening analysis for water soluble and bioavailable pollutants from running water.

The development of the new chemometric methods was mainly focused on a structured approach to GC-MS data analysis and on a systematization of these methods. The AMDIS software program, used for the deconvolution of mass spectra, played an important role in this study. The intelligent linking of several compound databases and chemical structure databases with AMDIS is vital for fast access to complete profiles (including physico-chemical properties, sources of chemicals and toxicity data) of the respective substances. A new approach was developed for metabolite analysis and identification. Metabolite databases and metabolite expert systems are coupled with AMDIS and the mass spectral search program. This lead to the identification of 15 DDT-metabolites in the SPMD samples. For an improved identification of substances, different expert systems were coupled: programs for the calculation of boiling points, for the detection of substructures from mass spectra, for the calculation of molecular masses and sum formulas, for the computation of connectivity isomers, and programs for substructure sorting. The benefit of coupling mass spectral data with Kovats- or Lee-retention indices was exemplified. The classification of GC-MS data with multivariate methods (principal component analysis, cluster analysis) can lead to an improved review process. The experimental data was visualized in 3D with the help of these multivariate methods. Furthermore, establishing an interdisciplinary and worldwide network for complete GC-MS profiles is likely to generate new synergies in environmental analysis.

This work contributed to the identification and characterization of ecotoxicologically relevant compounds. The suggested methods in this study can also be used in other fields like pharmaceutics or biosciences.