

# Benzoic Acid, Ibuprofen and Mecoprop in Danish Groundwater Samples: A Retrospective Quantification Study

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## Abstract

The accepted practise for monitoring the quality of groundwater is target analysis of pre-selected chemicals. Although they may still exist, chemicals not on the target list are ignored in this targeted approach. In a prior Non-Target Screening (NTS) study, groundwater samples from catchments with a variety of land uses were analyzed by Solid Phase Extraction, Dispersive Liquid-Liquid Micro Extraction with Gas Chromatography Mass Spectrometry analysis (SPE-DLLME-GC-MS). Potential chemical markers for land use, including benzoic acid (a natural metabolite), ibuprofen (a pharmaceutical) and mecoprop (a pesticide), were identified but not in this study, the detected chemical markers in SPE groundwater extracts that had been frozen for three years were retrospectively analysed and a strategy for retrospective quantitative analysis was developed. The preserved extracts underwent derivatization to change carboxylic acid. Detected, most likely from the dominant coniferous forest on this site. A possible method for tracking land use markers is the combination of NTS analysis and retrospective quantification. The NTS's lack of selectivity and storage effects make the technique difficult to implement method for preparing a sample. Derivatization and DLLME, two additional sample preparation procedures, were used in this study to increase the selectivity and sensitivity of the retrospective analysis.

**Keywords:** *Organozides; Photoredox catalysis; Lithium alkylamides; Dehydrogenative; Tetrasubstituted alkenes*

## Introduction

A pre selected list of compounds of interest is quantified as part of traditional target analysis of groundwater samples. While Non-Target Screening (NTS) analysis, which indiscriminately examines what is present in the sample, may identify novel chemicals of interest, it does not provide quantitative data. It would be possible to quickly quantify chemicals of new interest, such as chemical markers for land use and chemicals of rising concern, immediately from stored samples by combining NTS with retrospective quantitative analysis. However, because of the effects of storage and the lack of selectivity in standard NTS sample preparation techniques, such retroactive measurement may be problematic.

In a prior work, Solid Phase Extraction Dispersive Liquid-Liquid Micro Extraction Gas Chromatography Mass Spectrometry (SPE-DLLME-GC-MS) was used to analyse NTS groundwater. Benzoic acid was found at all 3 groundwater sites from the NTS study despite not previously being a focal compound in groundwater monitoring. Due to its high aqueous solubility and mobility in the soil column, benzoic acid is prone to seeping into the groundwater. The presence of iron and Aluminium oxides, in particular, can increase retention because benzoic acid forms surface complexes with these metal oxides, which can reduce mobility. There are numerous sources for benzoic acid, thus it is not surprising to find it in groundwater samples.

## Description

Benzoic acid was in groundwater samples from a former ammunition destruction site; however the source of the substance was not identified. Ibuprofen is an anti-inflammatory medication that is excreted into the sewer system. Pharmaceuticals like ibuprofen can enter the aquatic environment from wastewater treatment plants. Physical-chemical characteristics also have an impact on the concentration of pharmaceuticals in the aquatic environment. Ibuprofen concentrations were thereby positively connected with total dissolved solids, conductivity, salinity, total carbon, phosphate, sulphate, ammonium and negatively correlated with dissolved oxygen in lake water. The risk of ibuprofen leaching to groundwater is particularly significant in sandy,

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organic matter poor soils because soil ibuprofen absorption is restricted, but increases with levels of clay and organic matter and decreases with increasing pH. Mecoprop is a water soluble, mobile herbicide that has been linked to landfills, waste disposal sites, golf courses, horticultural and agricultural land uses as well as groundwater reservoirs. Like the two previous chemicals, mecoprop's ability to bind to soil depends on pH, clay content and organic matter levels. Mecoprop degrades significantly in topsoil, but less degrading is anticipated in the subsurface and the substance is quite stable in aquifers. Denmark's groundwater monitoring programmes routinely analyse mecoprop. In this investigation, the identified molecular markers benzoic acid, ibuprofen and mecoprop were retrospectively analysed in 60 SPE groundwater extracts that had been kept frozen. The target analytes were discovered in part as methyl esters since the SPE extracts had been kept in methanol under acidic conditions. Therefore, deuterated internal standards were spiked in the SPE extracts and treated by methanolic HCl derivatization under hot treatment to guarantee full derivatization in order to retrospectively quantify the target analytes. Seven tap water samples were also spiked with varied concentrations of benzoic acid, ibuprofen and mecoprop quantitation standards before being extracted by SPE using the same method as the 60 groundwater samples. After being spiked with internal standards, these extracts were additionally subjected to metabolic HCl derivatization before being used to create calibration curves.

## **Conclusion**

A combination of NTS analysis and retrospective quantification was used to quantify three chemical markers in Danish groundwater samples (benzoic acid, ibuprofen and mecoprop). After storage of a methanolic SPE extracts at -20°C for 3 years the method was able to reliably quantify the compounds. In contrast, the drug Ibuprofen and the pesticide mecoprop were only detected in a few sample wells indicating hot-spot contamination of the groundwater due to human activities.