

## Further Development of the Online Portal for Water Monitoring of the Future – Evaluation of Non-Target Screening Data for Environmental and Chemical Legislation (GdZ II)

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In contrast to conventional target analysis, non-target screening (NTS) does not pre-select substances. By using statistical methods, relevant anthropogenic signals are prioritized and then evaluated qualitatively (without specifying the concentration) or semi-quantitatively (estimation of the concentration via signal intensities). The NTS thus represents a central element for the future monitoring of water bodies, as anthropogenic substances can be analyzed and monitored more easily.

The aim of the project “Further development of the online portal for water monitoring of the future - evaluation of NTS data for environmental and chemical legislation (GdZ II)” is to develop approaches for the evaluation of NTS data in water monitoring (Figure 1).

In addition, professional and technical prerequisites for a permanent exchange of quality-assured data between the German Environment Agency (UBA) and the Federal Institute of Hydrology (BfG) will be created. This supports the environmental and chemical legislation as well as the German Centre for Micropollutants and other institutions in their work and serves as a template for data exchange in other NTS projects. To date, there has been a lack of the necessary approaches for data exchange, so that fundamental findings are to be collected between the two higher federal authorities UBA and BfG. The linking of relevant substance data (e.g. production volumes or toxicological information) and monitoring data (exposure) offers the possibility to create an assessment of the environmental behaviour of prioritized substances and substance mixtures. Subsequently, identified solutions for improving chemicals management can be proposed.

The central element of the GdZ is the NTS portal, which the BfG developed on behalf of the UBA in REFOPLAN FKZ 3720 222 010. It contains federal and state NTS measurements of suspended particulate matter and water samples and is both a database and a visualization platform. In the course of this project, possibilities will be created to make the portal easily accessible to interested users within the UBA.

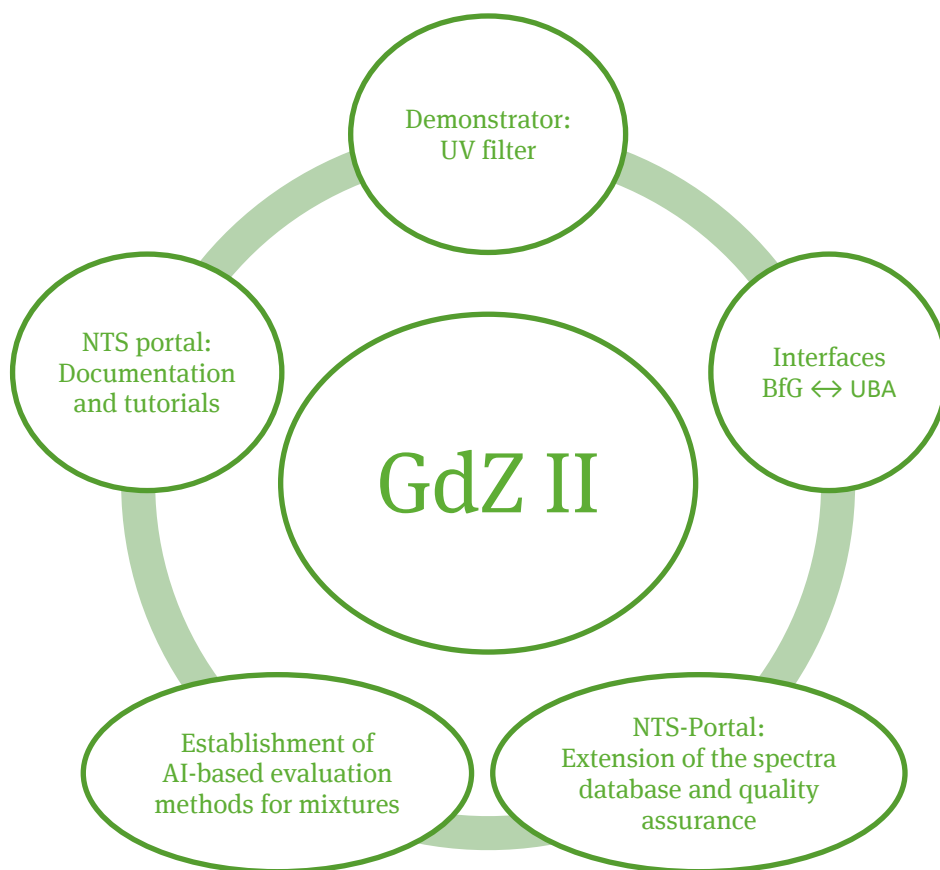


Figure 1: Schematic workflow in the project “Further development of the online portal for the water monitoring of the future - evaluation of NTS data for environmental and chemical legislation (GdZ II)”. Source: German Environment Agency.

A case study with the substance group of organic UV filters tests the analytical methods and workflows developed in the previous projects on a small scale. It was successfully demonstrated that NTS data from different laboratories can be combined and that the use of the NTS portal can provide important information on the behavior of substances in the environment. One advantage of non-target methods that should not be neglected is that they can focus on substances that were not prioritized and therefore not measured in previous target studies. These may also include toxicologically relevant degradation products.

The project is divided into five work packages. Work package 1 is based on the results of a master thesis prepared at the UBA (case study on UV filters). The other work packages aim at closely linking two higher federal authorities (BfG, UBA) and intend to demonstrate the applicability of the NTS portal on a large scale. Solutions are being developed in a doctoral thesis to characterize chemical mixtures using NTS data and to derive assessments of the environmental status from them.

The project is preceded by the following NTS projects at the UBA, the results of which are directly or indirectly incorporated into GdZ II:

- ▶ Methodology for the application of non-target screening (NTS) using LC-MS/MS in water monitoring (REFOPLAN FKZ 3717 22 230 0)
- ▶ Non-target screening in suspended matter and biota samples (REFOPLAN FKZ 3717 22 267 0)
- ▶ Online portal 'Non-target screening for the environmental monitoring of the future' (REFOPLAN FKZ 3720 22 201 0)
- ▶ Ad-hoc assessment in the water monitoring of the future (GdZ I, REFOPLAN FKZ 3722 22 201 1)

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