Introduction of the Project:
„ Non-Target Screening in the Rhine basin “

LUBW Landesanstalt für Umwelt Baden-Württemberg

LE GOUVERNEMENT DU GRAND-DUCHÉ DE LUXEMBOURG
Administration de la gestion de l'eau

BfG Bundesanstalt für Gewässerkunde

IKSR CIPR ICBR

Landesamt für Natur, Umwelt und Klima Nordrhein-Westfalen

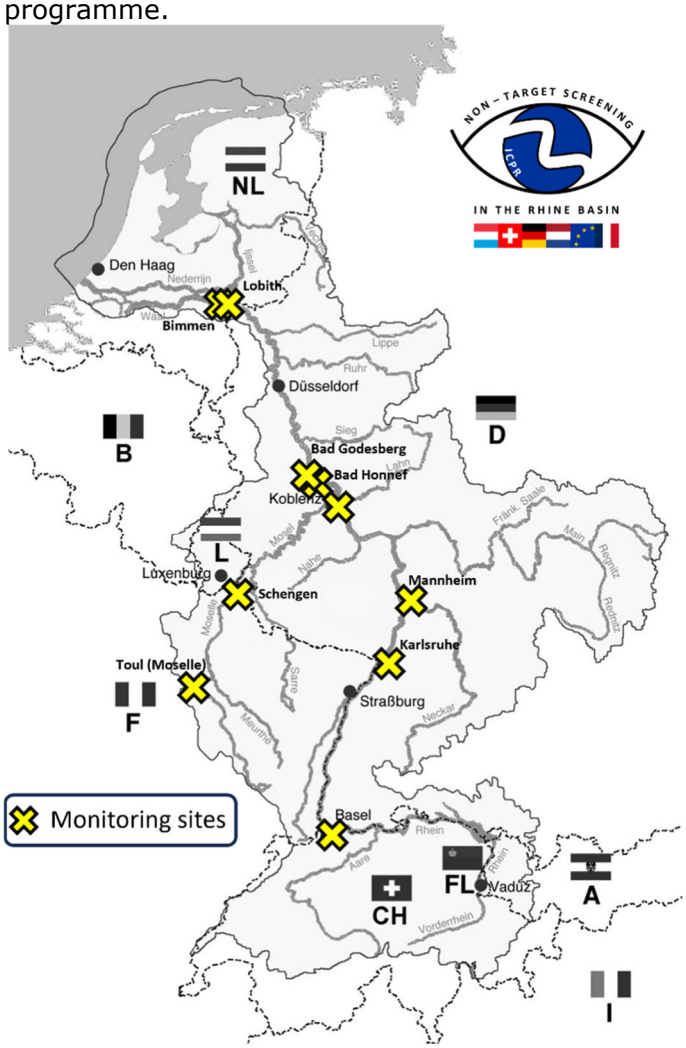
Rijkswaterstaat
Ministerie van Verkeer en Waterstaat

Departement für Wirtschaft, Soziales und Umwelt des Kantons Basel-Stadt
Amt für Umwelt und Energie

Géosciences pour une Terre durable
brgm

1 Project background

The "NTS in the Rhine Basin" joins the forces of several countries in the Rhine catchment (currently: Switzerland, Germany, France, Luxembourg and the Netherlands) to screen for suspected substances as well as to identify still unknown chemical substances in the river system. Using a harmonized approach by means of liquid chromatography coupled with high resolution mass spectrometry (LC-HRMS) and a shared "Cross Institutional Screening Database" (CIS-Database) enables all participating institutions and their laboratories to detect emerging pollutants more effectively.
The NTS Tool was developed as part of a pilot project running from 2021 to 2024 and partially funded via the EU-LIFE programme. Thanks to the success of the project, the project partners have decided to continue and further expand non-target screening in the Rhine River basin until at least 2029 and new project partners with additional monitoring stations have joined the project.
It aims at the routine use of harmonized NTS at 11 monitoring sites (see map), central data evaluation, and fast cross-border information exchange. This strengthens the scientific basis for water management and supports the goals of the "Rhine 2040" programme.



NTS provides daily insights into chemical composition, mission signals and their temporal trends, and new substances that may occur in the Rhine and its tributaries. Through the ICPR framework, these results are connected to relevant expert groups and integrated into international water governance, in particular the internationally coordinated River Basin Management Plan related to the EU Water Framework Directive.

2 Methods and Infrastructure

The approach is based on a harmonized liquid chromatography coupled with high resolution mass spectrometry (LC-HRMS method) applied across all participating laboratories and monitoring stations. The method uses a defined chromatographic regime, a fixed set of isotopically labeled internal standards, and recommended MS parameters to ensure comparability of data between laboratories. Daily composite and additional samples from the Rhine and its tributaries enable consistent detection of time-dependent trends, emission peaks, and emerging pollutants.
All measurement files generated in the participating laboratories are transferred via the BITBW Cloud to a central server at the LUBW. Here, the enviMass and the visualization tool (Vis-Tool) software processes, aligns, and aggregates the data. Core functions include peak detection, automated quality control, retention-time alignment across all labs, suspect screening through the CIS Database, and the extraction of compound emission profiles over time.
The Vis-Tool provides a unified interface to search for emerging pollutants across all stations (Figure 1), visualize temporal trends (Figure 2), inspect identified and unknown features (Figure 3-4), and exchange information between institutions (Figure 5). The system supports routine monitoring and the timely scientific evaluation of unusual or unexpected signals.

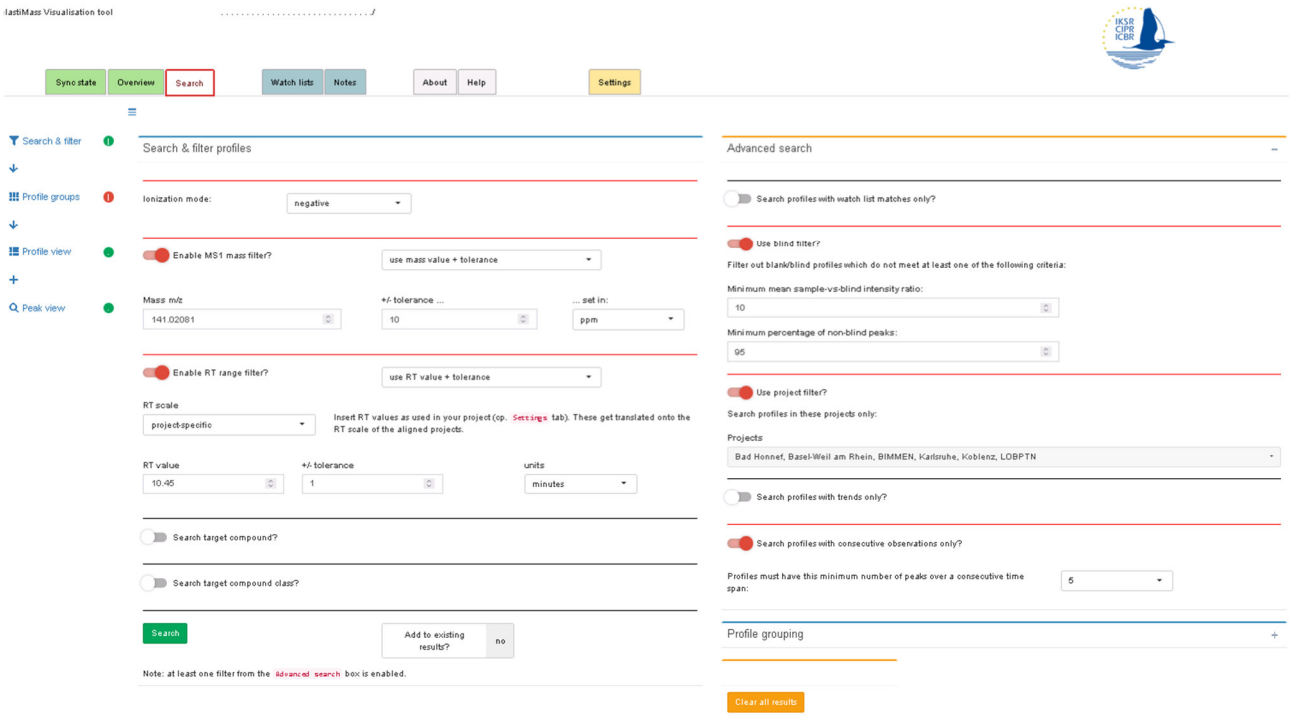


Figure 1 A Vis-Tool allowing to search for known and unknown chemicals across all involved monitoring sites.

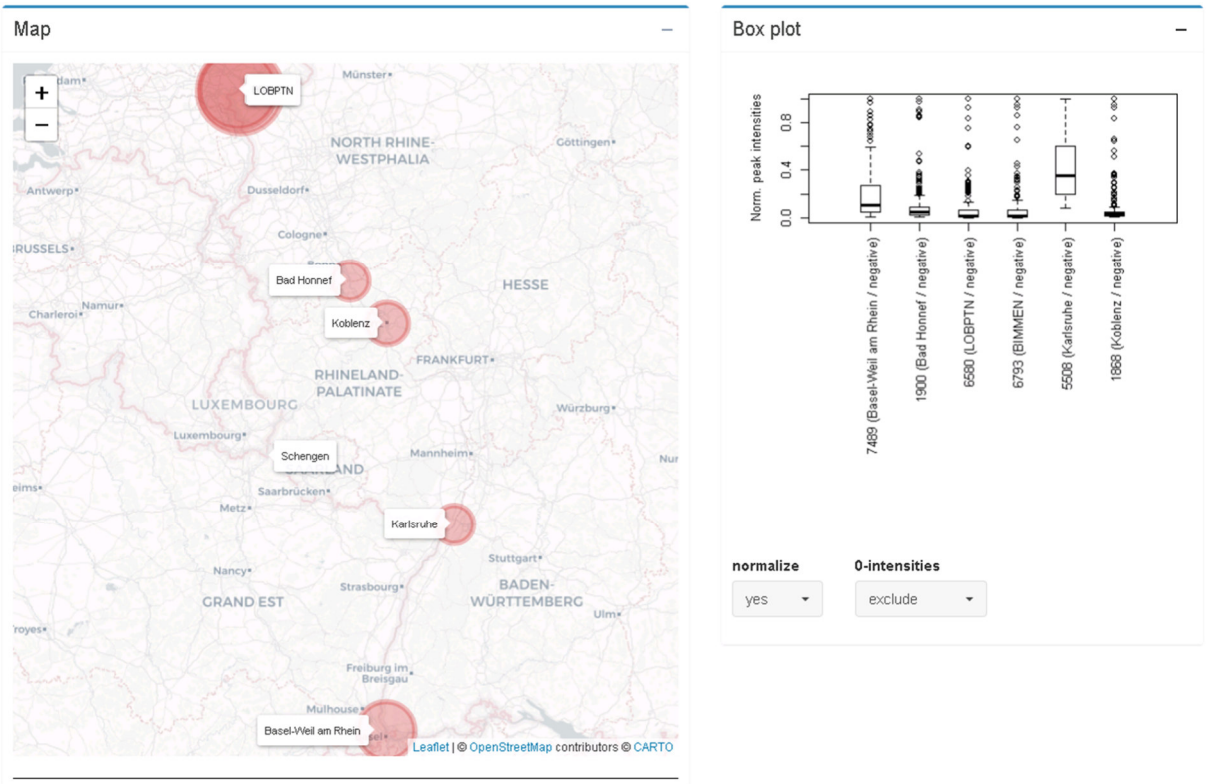


Figure 2 Map: occurrence of a searched compound on respective monitoring stations. The size of the red circles shows mean intensity rank. Box plot: normalized intensities detected at individual stations.

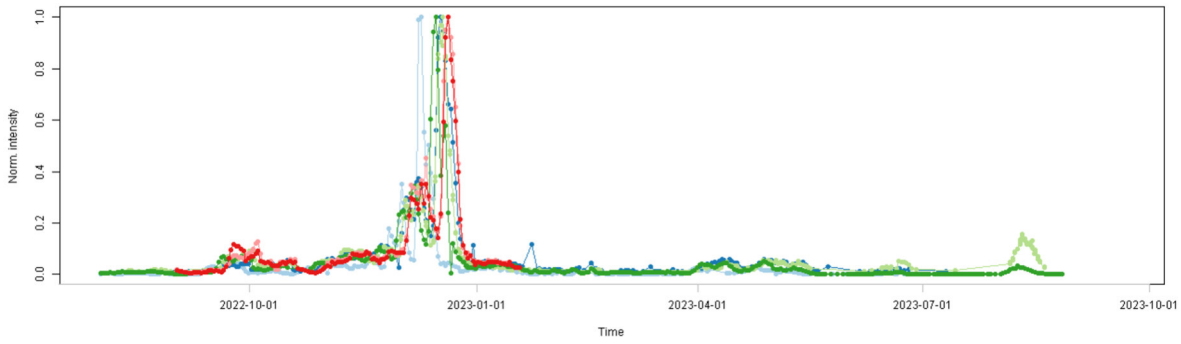


Figure 3 Example of mass profiles (2D view) found and displayed by means of the Vis-Tool.

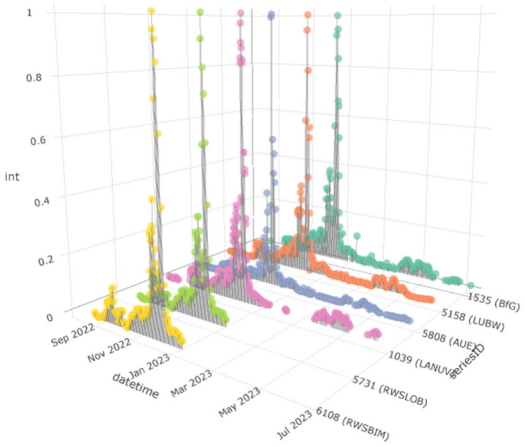


Figure 4 Example of mass profiles (3D view) found and displayed by means of the Vis-Tool.

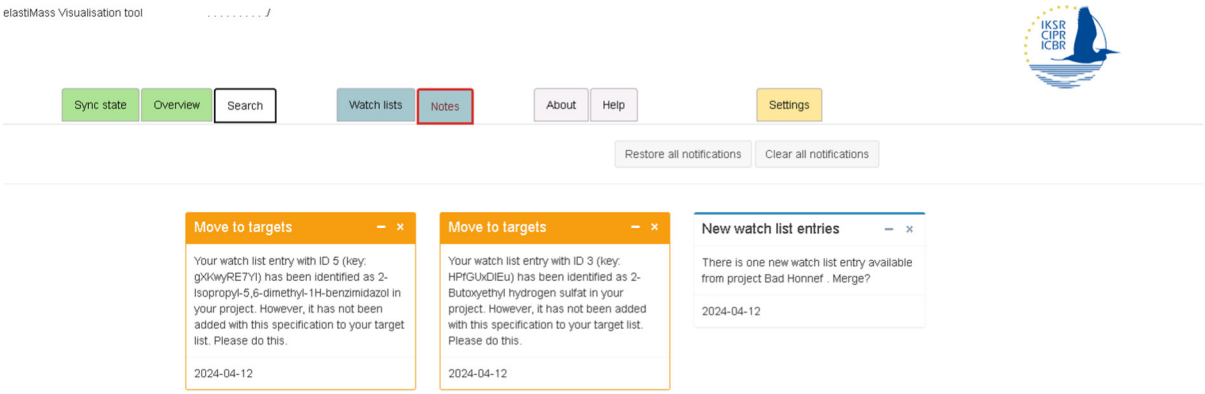


Figure 5 Notifications informs about newly identified emerging pollutants (orange) and Watch List entries (blue) that are followed by other laboratories or institutions.

3 International Cooperation

NTS in the Rhine Basin is a joint effort of environmental protection authorities and across several countries. The current cooperation is led by the ICPR and includes:

- Amt für Umwelt und Energie Basel-Stadt (AUE), Switzerland
- Bureau de recherches géologiques et minières (BRGM), France
- Landesanstalt für Umwelt Baden-Württemberg (LUBW), Germany
- Administration de la Gestion de l'Eau (AGE), Luxembourg
- Bundesanstalt für Gewässerkunde (BfG) in cooperation with Bundesministerium für Umwelt, Klimaschutz, Naturschutz und nukleare Sicherheit (BMUKN), Germany
- Landesamt für Natur, Umwelt und Klima Nordrhein-Westfalen, (LANUK), Germany
- Rijkswaterstaat (RWS), The Netherlands

In addition to the mentioned project partners, the Umweltbundesamt of the ICPR observer Austria is directly involved by data sharing.
The cooperation benefits from the ICPR framework, which brings together state delegations, environmental protection authorities, water suppliers (IAWR), and NGOs. Through shared workflows and common goals, NTS becomes a tool uniting the forces of the internation project partners.

4 Application in scope of IWAP and ICPR Expert Groups

The NTS Tool provides a detailed picture of chemical occurrence and temporal patterns in the Rhine system. It detects known substances and previously unrecognized chemical signals within the scope of the applied LC-HRMS instrumentation, supports long-term trend monitoring, and identifies short-term emission events that may originate from industrial, municipal, or agricultural sources.
The tool shall be further developed towards real-time monitoring. Already today, it supports the operation of the International Warning and Alarm Plan Rhine (IWAP). NTS enables faster recognition of substances that appear unexpectedly and supports the tracing of emissions along the river.
Within the ICPR structure, NTS provides input to several expert groups, including EG SANA (analytics), EG SMON (chemical monitoring), EG SAPA (international warning and alarm

plan), and EG SEMI (emissions). This ensures that scientific results from NTS can be used directly for monitoring, reporting, and water management decisions.

5 Future Development

During the follow-up phase (2024–2029), the NTS Tool will be expanded with several new capabilities. The CIS Database will continue to grow as laboratories add new identified substances and share knowledge on unknown features. Functions such as discharge-corrected trend analysis, integration of NTS based on gas chromatography coupled with mass spectrometry (GC-MS), and improved toxicity-related evaluation are planned.
Further development will also focus on strengthening information exchange with other screening databases in Europe, improving quantification approaches, and providing better tools for prioritizing substances. An increasing number of institutions using the Vis-Tool or connected via InfoShare will improve the understanding of NTS results and raise the overall level of knowledge within the network.
The long-term goal is to embed NTS as a stable component of international environmental monitoring in the Rhine Basin. Through ongoing cooperation, harmonized methods, and centralized data evaluation, NTS will continue to improve the understanding of chemical pollution and support evidence-based water protection across borders.