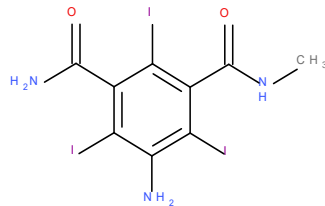




5-Amino-2,4,6-triiodo-N-methylisophthalamide

5-Amino-2,4,6-triiodo-N-methylisophthalamide is a previously unknown substance in surface waters. It has a symmetrically substituted triodobenzene ring. Many known iodinated X-ray contrast media also have this basic structure. 5-Amino-2,4,6-triiodo-N-methylisophthalamide appears to be formed in wastewater treatment plants and not in the production of X-ray contrast media.

Molar mass:
570.7751 g/mol
CAS: -
C₉H₈I₃N₃O₂



The measurements of the LANUV meet the following necessary criteria for clear identification:

- 1) Match of the exact mass, ± 5 ppm
- 2) Match of the isotope pattern, min. 70 %
- 3) Match of a reference spectrum
- 4) Match of the retention time with the reference substance

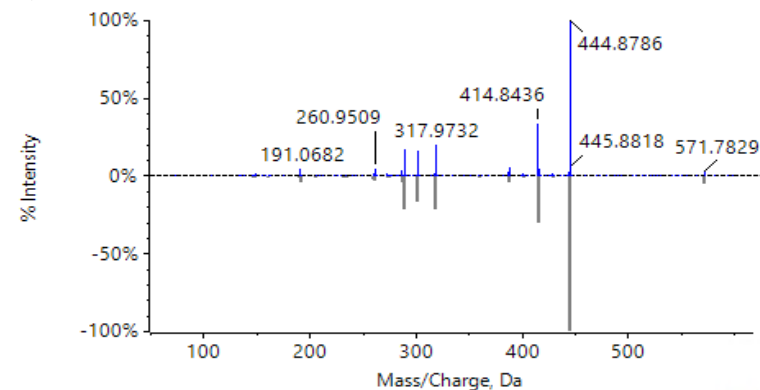


Figure 1: comparison of fragment-ion-spectra, blue: sample river Lippe Wesel, grey: reference substance

Analytics and occurrence

During regular non-target-screening, an unknown signal with a mass-to-charge ratio of m/z 571.7820 was repeatedly detected in the river Lippe near Wesel. The unknown substance could be detected in positive mode with the existing measuring method. The river Rhine was sampled at different Rhine kilometers (right, left and middle). Figure 2 clearly shows that m/z 571.7820 is only detectable from Rhine km 837 and has significantly higher signals in the right and middle Rhine samples. Therefore, the discharge of the substance via the river Lippe is very likely (confluence with the river Rhine at Rhine km 814).

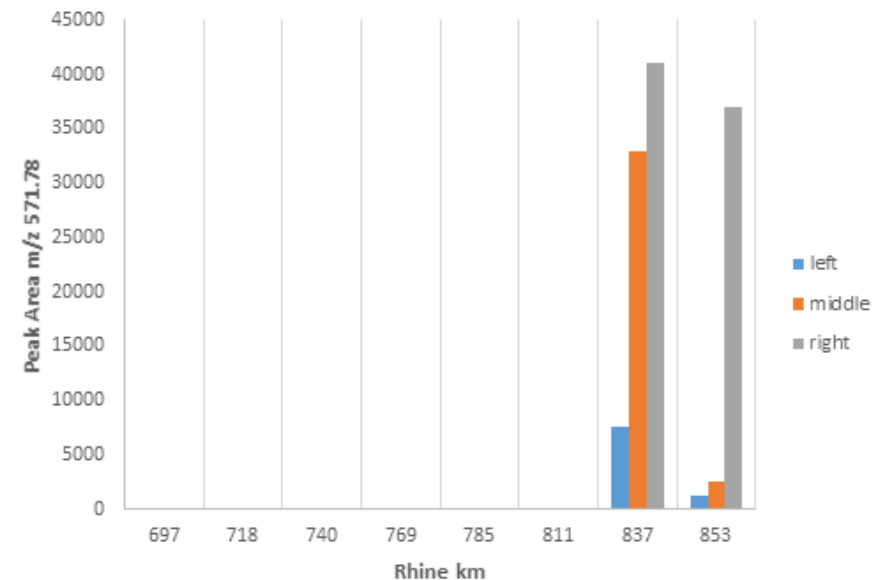


Figure 2: Cross profile river Rhine September 2022



The river Lippe was then sampled to identify one or more dischargers. After a short time, a discharger was identified. After discussions and mutual exchange of information, the unknown was identified using a synthesized standard. The unknown is 5-amino-2,4,6-triiodo-N-methylisophthalamide. Figure 3 shows the concentration of 5-amino-2,4,6-triiodo-N-methylisophthalamide from June 2023 to January 2024 with the corresponding discharge of the river Lippe at Dorsten.

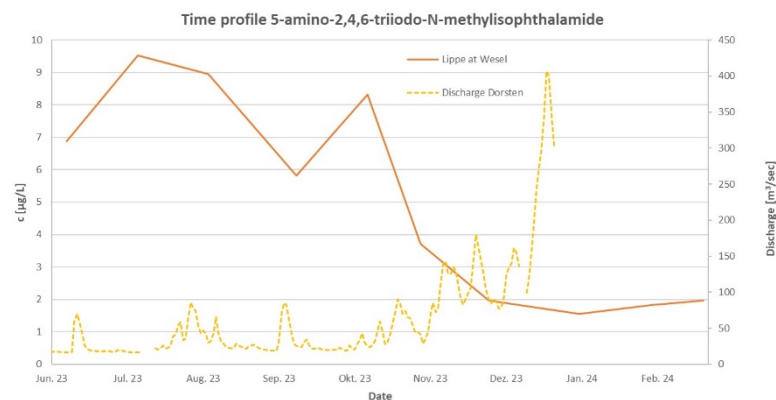


Figure 2: Time profile of 5-Amino-2,4,6-triiodo-N-methylisophthalamide in the river Lippe at Wesel

The general prevention value of 0.1 µg/L is clearly exceeded in the Lippe near Wesel (max. 9.5 µg/L), concentrations of max. 0.3 µg/L were measured in the river Rhine at Lobith. 5-Amino-2,4,6-triiodo-N-methylisophthalamide was not detected in the river Ruhr, Wupper, Emscher and Ems.

Relevance

There are no legally binding limit values for 5-amino-2,4,6-triiodo-N-methylisophthalamide in drinking water. Therefore, the general prevention value of 0.1 µg/L is used for assessment. No substance properties or data on behaviour in drinking water treatment can be researched for the substance. Therefore, an assessment of drinking water relevance is not possible at this time.

For 5-amino-2,4,6-triiodo-N-methylisophthalamide no ecotoxicological data can be researched. An assessment of aquatic biocenosis relevance is not possible due to lack of data. Modelling data from EPI Suite™ 4.1 indicate that the substance is not readily biodegradable.

Further procedure:

There is intensive contact with the discharger. The district government has been informed and discussions are underway with the discharger to minimize the discharge. The river Lippe is still being sampled.