



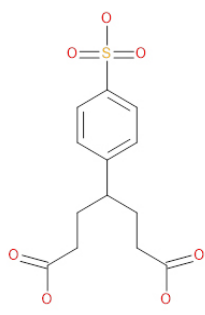
4-(4-Sulfophenyl)heptanedioic acid

4-(4-Sulfophenyl)heptanedioic acid belongs to the sulfophenyl-di-carboxylates (SPdCs). Not much is known about its use due to insufficient data. It is assigned to the group of surfactants and is described as a degradation product of linear alkylbenzenesulfonates (LAS).

mass: 316.33 g/mol

CAS: -

$C_{13}H_{16}O_7S$



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

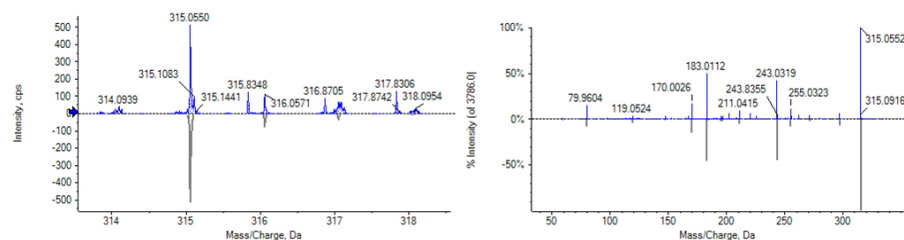


Figure 1: left: comparison of isotope patterns, blue: Rhine sample near Bad Honnef, grey: theoretical isotope pattern; right: comparison of fragment-ion-spectra, blue: sample Rhine near Bad Honnef, grey: reference substance

Analytics and occurrence

4-(4-Sulfophenyl)heptanedioic acid can be detected with the existing measuring method in negative mode. It could be detected with different intensity in almost all investigated rivers (Rhine, Sieg, Ruhr, Emscher, Lippe) and therefore belongs to the ubiquitous substances.

In the Rhine, the concentration of 4-(4-Sulfophenyl)heptanedioic acid increases during the winter months and decreases again in the summer months, a clear influence of the discharge could not be observed over the last three years. It could possibly be a seasonal input or a production-related increase. In the Rhine, the average concentration of the background exposure is $0.1 \mu\text{g/L}$ and increases by at least a factor of five during the winter months (see Figure 2).

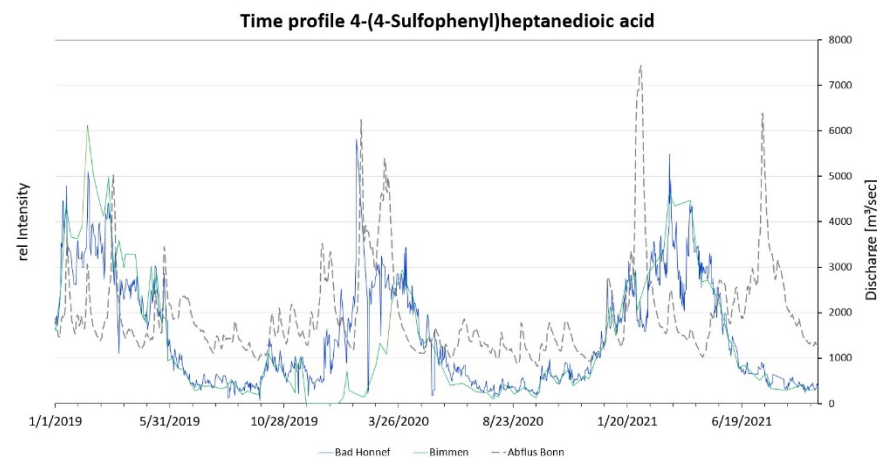


Figure 2: Time profile 2019-2021 of 4-(4-Sulfophenyl)heptanedioic acid in the Rhine near Bad Honnef and Bimmen with discharge¹ at Bonn

¹ Federal Waterways and Shipping Administration (WSV), provided by the Federal Institute of Hydrology (BfG). This applies to first, second and any subsequent use.



Individual measurements of the Rhine between kilometers 697 to 852 show that the Emscher causes a short-term increase in concentrations in the Rhine.

Relevance

There are no legally binding limit values for 4-(4-Sulfophenyl)heptanedioic acid in drinking water. Therefore, the general precautionary value of 0.1 µg/L for drinking water is used for the assessment. So far, no information on the behavior in drinking water purification is available. Due to no specific data on substance properties and toxicity, no assessment in regard to drinking water relevance is possible.

There are no ecotoxicological data available for the substance. The modeled log P does not indicate an increased bioaccumulation potential. Data to assess the persistence of 4-(4-Sulfophenyl)heptanedioic acid are not available.

Further procedure:

4-(4-Sulfophenyl)heptanedioic acid belong to the ubiquitous substances, because it could be detected in all of the investigated surface waters. Despite the inputs by the various tributaries, the comparison of the time courses at the measuring station in Bad Honnef (inflow of the Rhine in NRW) and in Bimmen (end of the Rhine in NRW) indicates that there is no significant impact on the background exposure of the Rhine.

In order to determine a possible discharger and to clarify the increase in the background exposure during the winter months, further measurements are planned for the corresponding period.