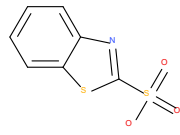




## Benzothiazole-2-sulfonic acid

Benzothiazoles consist of a benzene ring and a thiazole ring, both rings can be substituted. This results in a wide variety of derivatives. The derivatives are mainly used in tire production as vulcanization accelerators. Some of these substances can be converted to benzothiazole-2-sulfonic acid in aqueous medium.

mass: 215.25 g/mol  
CAS: 941-57-1  
C<sub>7</sub>H<sub>5</sub>NO<sub>3</sub>S<sub>2</sub>



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

- 1) Match of the exact mass,  $\pm 5$  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

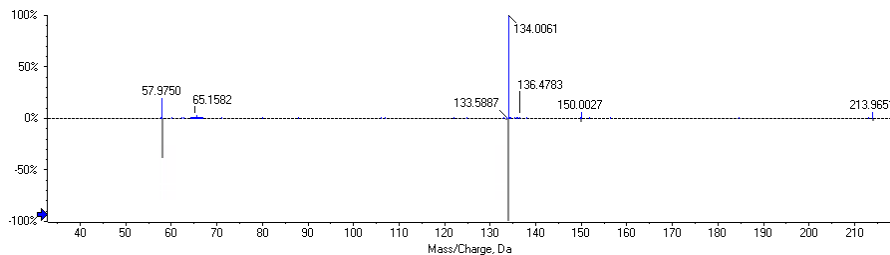


Figure 1: Comparison of fragment-ion-spectra, blue: sample Ruhr near Mülheim, grey: reference substance

## Analytics and occurrence

Benzothiazole-2-sulfonic acid can be detected in negative mode with the existing measuring method. It was found in all investigated rivers (Rhine,

Ruhr and Ems) and is therefore a ubiquitous substance. The concentrations are mostly between 0.1 - 2.5  $\mu\text{g/L}$ .

## Relevance

There are no legally binding limit values for benzothiazole-2-sulfonic acid in drinking water. Therefore, the general prevention value of 0.1  $\mu\text{g/L}$  for drinking water is used for the assessment. Due to its substance properties (polar, mobile, poorly biodegradable, remains in the water phase, low bioaccumulation potential), the substance is classified as potentially relevant to drinking water based on the data available. Due to the polarity of the substance, the removability of benzothiazole-2-sulfonic acid within drinking water treatment has to be investigated.

No ecotoxicological data are available for benzothiazole-2-sulfonic acid. Due to the low log P, no high bioaccumulation potential is expected.

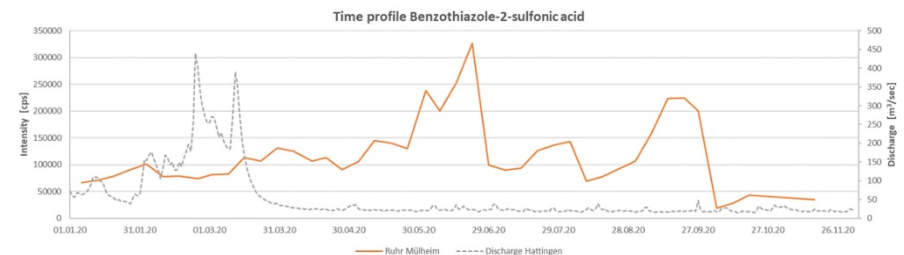


Figure 2: Time profile of benzothiazole-2-sulfonic acid in the Ruhr near Mülheim <sup>1</sup>

## Further procedure:

Benzothiazole-2-sulfonic acid is ubiquitous and consistently occurs at comparable concentrations between 0.1 and 2.5  $\mu\text{g/L}$ . It exceeds the prevention value of 0.1  $\mu\text{g/L}$  regularly. Because vulcanization accelerators often contain metals, a possible correlation should be investigated in a project.