Non Target – News #11

Landesamt für Natur,
Umwelt und Verbraucherschutz
Nordrhein-Westfalen

Chlorothalonil metabolites

The following chlorothalonil metabolites were investigated:

Name	Molecular formula
Chlorothalonil metabolite R417888	$C_8H_3Cl_3N_2O_4S$
Chlorothalonil metabolite R471811	$C_8H_5Cl_3N_2O_5S$
Chlorothalonil metabolite R611968	$C_8H_3Cl_3N_2O_2$
Chlorothalonil metabolite SYN507900	$C_8H_3Cl_3N_2O_2$
Chlorothalonil metabolite SYN548580	$C_8H_5Cl_3N_2O_3$
Chlorothalonil metabolite SYN548581	$C_8H_3Cl_3N_2O_4S$

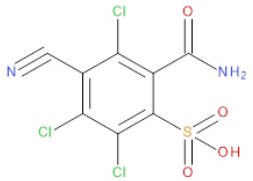
Table 1: Overview of investigated metabolites

In the following, the most relevant chlorothalonil metabolites (chlorothalonil metabolite R417888 and chlorothalonil metabolite R471811) according to Kiefer et al. (2019) were investigated in more detail. For the remaining four metabolites, there were no results in the tested samples (LOQ 0.025 µg/L).

Chlorothalonil metabolite R417888

mass: 329.54 g/mol

$C_8H_3Cl_3N_2O_4S$

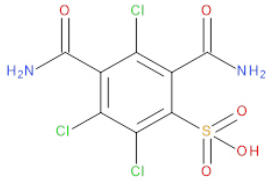


[1] New Relevant Pesticide Transformation Products in Groundwater Detected Using Target and Suspect Screening for Agricultural and Urban Micropollutants with LC-HRMS, Karin Kiefer, Adrian Müller, Heinz Singer, Juliane Hollender

Chlorothalonil metabolite R471811

mass: 347.56 g/mol

$C_8H_5Cl_3N_2O_5S$



Chlorothalonil metabolite R417888 and chlorothalonil metabolite R471811 are metabolites of the broad-spectrum fungicide chlorothalonil. It was registered for use in 1966, but is banned in the EU since May 2020.

The LANUV measurements meet the following criteria necessary 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 retention time

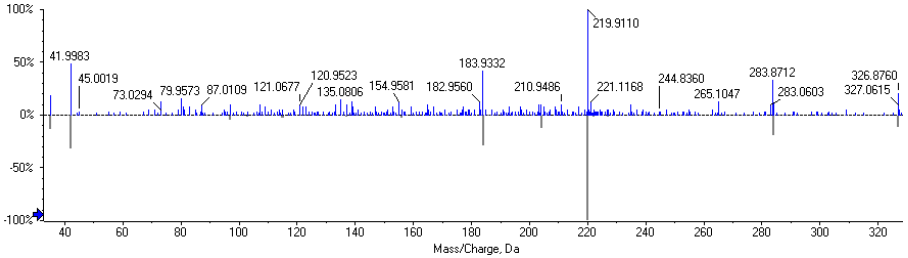


Figure 1: comparison of fragment-ion-spectra, blue: sample Lippe near Wesel, gray: reference substance (R417888)

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Analytics and occurrence

Chlorothalonil metabolite R417888 can be detected with the existing measurement method in negative mode. For Chlorothalonil metabolite R471811, the method is not well suitable. The concentrations for Chlorothalonil metabolite R417888 were below 0.1 µg/L in the investigated rivers (Rhine, Ruhr and Lippe).

Relevance

According to the "GOW list" of the UBA (November 2021)[2] , the chlorothalonil metabolite R471811 is a non-relevant metabolite for which a GOW of 3.0 µg/L is specified. The substance is expected to be persistent in the water phase because of a low log Kow value and its slow degradation[3] . The removal of chlorothalonil and its metabolites is usually achieved by reverse osmosis is considered to be well capable. Other processes such as activated carbon, UV disinfection or ozonation are unsuitable or restricted applicable[4] . Recent research results with a filter material based on activated carbon show very good results for the removal of chlorothalonil and its metabolites[5] . Based on the data available, the substance is classified as potentially relevant to drinking water.

No ecotoxicological data are available for the substances. Due to the low log P, no high bioaccumulation potential is expected. The available data indicate that the substance is persistent in the environment

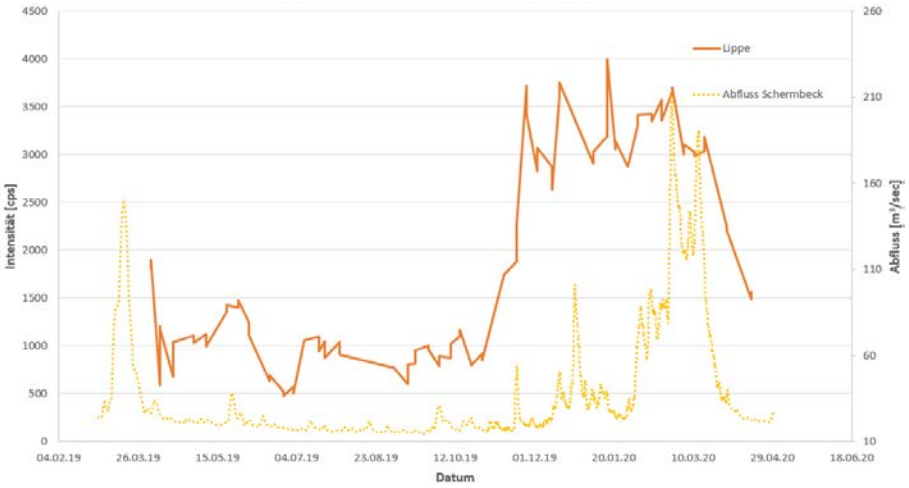

Figure 2: Time profile of chlorothalonil metabolite R417888 in the Lippe near Wesel

Further procedure:

A new measuring method will be developed so that reliable results can also be given for chlorothalonil metabolite R471811. Results are available here:

- https://www.lanuv.nrw.de/fileadmin/lanuv/analytik/pdf/echo/ECHO_News__Chlorthalonil-Metabolite_2021eng.pdf

[2] https://www.umweltbundesamt.de/sites/default/files/medien/5620/dokumente/gowpflanzenschutzmetabolite-20211109_0.pdf

[3] EFSA (European Food Safety Authority), 2018. Conclusion on the peer review of the pesticide risk assessment of the active substance chlorothalonil. EFSA Journal 2018;16(1):5126, 47 pp. doi:10.2903/j.efsa.2018.5126 – Appendix A

[4] https://www.eawag.ch/fileadmin/Domain1/Beratung/Beratung_Wissenstransfer/Publ_Praxis/Faktenblaetter/fb_chlorothalonilmetaboliten_d.pdf

[5] https://www.uwiag.com/biogreenp