

Abstract

The occurrence of pharmaceuticals in aquatic systems is of concern for environmental assessment. Often, elimination in municipal wastewater treatment plants is incomplete and results in the release of pharmaceutical residues to the aquatic environment. While the presence of drugs in the aquatic environment is the topic of many studies, information on the corresponding ecotoxicity, persistence and fate of pharmaceuticals and their transformation products in the environment are scarce.

The analgesic, anti-arthritic and anti-rheumatic pharmaceutical diclofenac (DCF) is one of the most common pharmaceutical products identified in surface and groundwater. DCF is only partly eliminated by water treatment plants, with a removal efficiency of 0 – 75% and thus might pose a potential risk to drinking water resources. Moreover, photolysis was reported to be the most important transformation pathway of DCF in surface waters leading to a transformation of up to 90% of the DCF within a few hours. Photo-transformed DCF were reported to be 5 times more toxic to green algae compared to the parent compound.

The aim of this EDA study was the identification and subsequent confirmation of the DCF photo-transformation product causing the enhanced toxicity standard solution of DCF with simulated sunlight, reversed-phase high performance liquid chromatography (HPLC) fractionation of photo-transformation products, effect assessment using reproduction inhibition of the green algae *S. vacuolatus* and chemical analysis of biologically active fractions using HPLC and gas chromatography / mass-spectrometry. Special focus was given on structure elucidation applying state-of-the-art computer tools and on the confirmation of the toxic product as suggested previously.

We identified and subsequently confirmed 2-[2-(chlorophenyl)amino]benzaldehyde (CPAB) as a transformation product with enhanced toxicity using effect-directed analysis. The EC_{50} of CPAB (4.8 mg/L) was a factor of 10 lower than that for DCF (48.1 mg/L), due to the higher lipophilicity of CPAB (log Kow = 3.62) compared with DCF (log Dow = 2.04) at pH 7.0.

In conclusion, effect-directed analysis of irradiated diclofenac resulted in the identification of one photo-transformation product responsible for the enhanced toxicity to *S. vacuolatus*. The compound seems to be at least as persistent in the environment due to the permanent release of DCF. Thus it should be included in monitoring and risk assessment of pharmaceuticals in the environment.

Veröffentlicht als:

Schulze, T.; Weiss, S.; Schymanski, E.; Von der Ohe, P. C.; Schmitt-Jansen, M.; Altenburger, R.; Streck, G. & Brack, W. (2010): Identification of a phytotoxic photo-transformation product of diclofenac using effect directed analysis; Environ Pollut 158, 1461–1466 (<http://dx.doi.org/10.1016/j.envpol.2009.12.032>)