Assessment of previously unknown anthropogenic trace contaminants

RISK-IDENT

The project RISK-IDENT develops and applies an identification system for both - already known and so far unknown - anthropogenic trace contaminants occurring in aquatic environments. In addition to the risk assessment of selected (newly identified) trace contaminants – including the formation of metabolites and the protection of drinking water resources – a new method for eliminating trace contaminants during waste water treatment will be tested. The results will be allocated as instruction guidelines for the identification and risk management of unknown trace contaminants.

A customized knowledge transfer of the project results to the target groups municipalities, citizens and economy provides a basis for decision-makers and new concepts for further education.

database STOFF-IDENT for the identification of unknowns and knowns

- obligatory features:
  - CAS-number
  - molecular formula ← exact mass
  - chemical name
  - Log P and Log D when applicable
  - pKa
  - chemical group or application
  - data source
  - additional information:
    - water solubility
    - Kp and Koc
    - R50/R53 classification

RISK-IDENT comprises data sets for potentially trace contaminants in water:
- REACH-registered chemicals (High-volume >1000 tonnes per year; chemicals with R50/R53 label, CMR chemicals category 1 and 2 with >1 tonne per year)
- registered pesticides and their metabolites
- registered pharmaceuticals and their metabolites
- registered biocides
- substance lists from prioritisation processes (e.g. NORMAN list of emerging pollutants)
- pollutants found in research projects and monitoring programmes (e.g. artificial sweeteners, corrosives etc.)
- probable transformation products derived from prediction systems (e.g. Univ. of Minnesota Pathway Prediction System UM-PPS, CATALOGIC, ZENETH) after checking stability using EPISuite™ 4.10/BIOWIN™
- union of databases or programmes

RISK-IDENT

retention time index (RTI)

- normalisation of retention times with known logP/logD data using a software developed by a project partner (openMASP.hswt.de)
- use of about 10 retention time markers enables the comparability of chromatographic conditions used in different laboratories
- May - July 2012: interlaboratory test with defined solutions for LC-separations with C18 reversed-phase-materials (contact: T.Letzel@wzw.tum.de)

non-target-screening with LC-HRMS

- check with STOFF-IDENT → substance proposals
- check proposals with retention time index
- analysis of proposed and measured fragments
- check plausibility with additional data
- confirmation of structure by reference substances

example: valsartan in waste and surface waters

- elimination of the angiotensin II receptor antagonist valsartan is investigated in lab-scale WWTPs at 1 – 50 µg/l for up to 28 days
- average elimination rate 97%
- LM-PPS combined with BIOWIN™ proposes 24 stable transformation products
- exact mass and logP™ calculated
- LC-TOF-MS analysis of effluent samples to identify transformation products and
- LC-TOF-MS analysis of real WWTP effluents and surface water
- exact mass of predicted transformation product valsartan acid found in lab-scale WWTPs, real waste water and surface water
- identification of further transformation products in progress
- ecotoxological studies (daphnia magna 21-d reproduction test; green algae-growth inhibition test; Ames fluctuation test) of lab-scale WWTP effluents are performed to estimate the toxicity of transformation products