RISK IDENT Identifizieren | Bewerten Handeln | Kommunizieren

# Assessment of previously unknown anthropogenic trace contaminants

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## 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 and a database of potential as well as identified anthropogenic trace contaminants will be elaborated. 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

**comprising data sets for potentially trace contaminants in water:**

- REACH-registered chemicals (high-volume >1000 tonnes per year; chemicals with R50/53 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™
- …

**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
- $K_H$ and $K_D$
- R50/R53 classification

STOFF-IDENT

**connection to other databases or programmes**

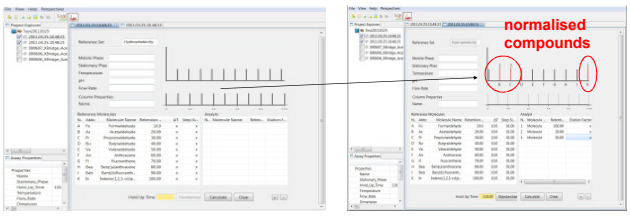
- DAIOS
- NORMAN MassBank
- Chemspider
- MetFrag
- …

- after end of project yearly update with new REACH entries by LfU
- free access via web

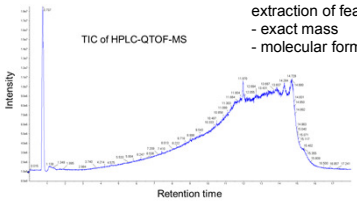
## retention time index (RTI)

| | Retentionszeit (RT) | | | logP | | | | | logD | |
|---|---|---|---|---|---|---|---|---|---|---|
| | Langenau | LfU | TUM | Sigma | pubchem | Tomlin | chemicalize.org | ACD | pH 7.4 | Marvin pH 7.4 |
| Standardname | | | | logP | logP | logP | logP | logP | logD | logD |
| Carbendazim | 7.3 | 8.92 | 10 | 1.5 | 1.5 | 1.51 | 2.02 | 1.52 | 1.49 | 1.8 |
| Carbetamide | 8.8 | 14.5 | 11.8 | k.A. | 1.6 | k.A. | 1.65 | 1.52 | 1.52 | 1.65 |
| Prosulfocarb | 16.9 | 21.3 | 20.1 | k.A. | 3.9 | 4.65 | 4.17 | 3.99 | 3.99 | 4.17 |

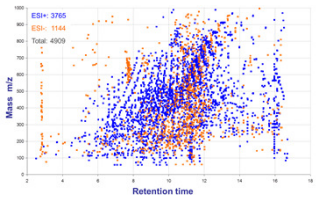
- normalisation of retention times with known logP/logD data using a new software developed by a project partner (openMASP.hswt.de)
- use of about 10 retention time markers enables the comparability of chromatographic conditions used in different laboratories
- May - July 2012: interlaboratory test with defined solutions for LC-separations with $C_{18}$ reversed-phase-materials (contact: T.Letzel@wzw.tum.de)




## non-target-screening with LC-HRMS




extraction of features
- exact mass
- molecular formula



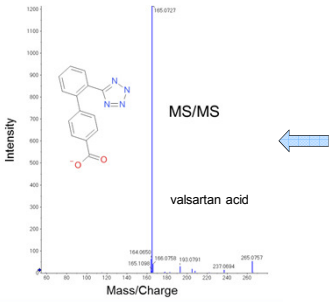

check with STOFF-IDENT → substance proposals

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%
- UM-PPS combined with BIOWIN™ proposes 24 stable transformation products
- exact mass and logP calculated

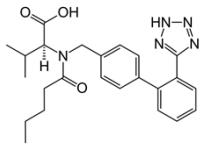
- LC-TOF-MS analysis of effluent samples to identify transformation products

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

ecotoxicological 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



valsartan, CAS-Nr 137862-53-4

valsartan acid, CAS-Nr 164265-78-5
(see also Kern at al. 2010)

More information: http://risk-ident.hswt.de http://www.riskwa.de

Kern S. et al., J.Environ.Monit., 2010, 12, 2100-2111

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