

A decorative graphic on the left side of the slide consisting of a network of light blue circles connected by lines, resembling a molecular or biological pathway.

Data elements and packages in enviPath

Jasmin Hafner

Kathrin Fenner

11 May 2025

Overview

1. Data organization in enviPath
2. Data packages in enviPath
3. Navigating enviPath data



Universität
Zürich^{UZH}

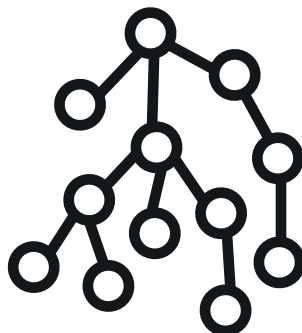
enviPath - a platform for environmental contaminant biotransformation

envipath.org



Database

Biodegradation data – pathways, half-lives, experimental conditions



Pathway prediction engine

Predicts biotransformation pathways and products

enviPath

Package Pathway Rule Compound Reaction Relative Reasoning Scenario Setting User Group Search Info Login

enviPath | THE ENVIRONMENTAL CONTAMINANT BIOTRANSFORMATION PATHWAY RESOURCE

enviPath is a database and prediction system for the microbial biotransformation of organic environmental contaminants. The database provides the possibility to store and view experimentally observed biotransformation pathways. The pathway prediction system provides different relative reasoning models to predict likely biotransformation pathways and products. You can try it out below.

[Learn more >>](#)

SMILES [Go!](#)

Twitter

Follow @enviPath

Tweets by @enviPath

enviPath Retweeted
Sebastian Schmidt @SebSchChem
Our paper on the holistic evaluation of predicted biodegradation/metabolism pathways with our partners @enviPath @MLAucklandUni appeared in @jcheminf. Dealing with problems like transient intermediates that are missing in the experimental reference data, or multi-step reactions. <https://twitter.com/jcheminf/status/1434041421393182721>

Sep 4, 2021

enviPath Retweeted
Journal of Cheminformatics @jcheminf
new: "Holistic evaluation of biodegradation pathway prediction: assessing multi-step reactions and intermediate products" jcheminf.biomedcentral.com/articles/10.11...

News

Tutorial
Mon, 05 Oct 2020 10:07:08 +0000
We recently prepared four tutorial videos. They cover basic functionality such as the data model, data access, pathway creation, and pathway prediction. Check them out...

enviPath Updates
Mon, 06 Jul 2020 09:25:56 +0000
We did not post any news for quite a while, but a lot has happened in the recent months, and enviPath has progressed quite a...

License
Tue, 18 Jun 2019 08:38:42 +0000
The core data sets of enviPath are licensed under the Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International (CC BY-NC-SA 4.0) license. This allows you to use them...

Update - July 7, 2016
We just deployed another update, most changes are on a lower level. Some important updates are: Introduction of multiple structures for one compound, updates in relative reasoning (more updates on this will come in the next month), introduction of a mapping servlet to map PPS rules to enviPath URIs, and

Latest Pathway

Technetium Immobilization

enviPath 101

Wiki
The main documentation can be found [in our wiki](#).

enviPath Tutorial: Pa...

eawag
aquatic research

THE UNIVERSITY OF
AUCKLAND
SCHOOL OF COMPUTER SCIENCE
MACHINE LEARNING

THE UNIVERSITY OF
AUCKLAND
SCHOOL OF COMPUTER SCIENCE
MACHINE LEARNING

SCIENCE
SCHOOL OF COMPUTER SCIENCE
MACHINE LEARNING

[Impressum/Imprint](#)

[Contact](#)

enviPath UG (haftungsbeschränkt) & Co. KG © 2022

1. Data organization in enviPath

Where does the biodegradation data come from ?

Scientific literature and regulatory reports

Renewal Assessment Report

28 February 2014

Isoproturon

Volume 3

Annex B.8

Environmental fate and behaviour

RMS: Germany **Co-RMS: Czech Republic**



1,3-DICHLOROPROPENE

of the second stage of the review programme referred to in Article 8(2) of Council Directive 91/414/EEC

Volume 3, Annex B, part 5, B.7 – B.9

November 2004

Environmental Science & Technology

Article
pubs.acs.org/est

Systematic Exploration of Biotransformation Reactions of Amine-Containing Micropollutants in Activated Sludge

Rebekka Gulde,^{1,2} Ulf Meier,¹ Emma L. Schymanski,¹ Hans-Peter E. Kohler,^{1,2} Damian E. Helbling,³ Samuel Derrer,¹ Daniel Rentsch,¹ and Kathrin Fenner^{1,2,3}

¹Eawag, Swiss Federal Institute of Aquatic Science and Technology, 8600 Dübendorf, Switzerland
²Department of Environmental Systems Science (D-USYS), ETH Zürich, 8092 Zürich, Switzerland
³School of Civil and Environmental Engineering, Cornell University, Ithaca, New York 14853, United States
⁴EMPA, Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland

Supporting Information

ABSTRACT: The main removal process for polar organic micropollutants during activated sludge treatment is biotransformation, which often leads to the formation of stable transformation products (TPs). Because the analysis of TPs is challenging, the use of pathway prediction systems can help by generating a list of suspected TPs. To complete and refine pathway prediction, comprehensive biotransformation studies for compounds exhibiting pertinent functional groups under environmentally relevant conditions are needed. Because many polar organic micropollutants present in wastewater contain



structurally diverse primary, elucidation of 101 of these the highest relevance were N- acetylation were similar to those actions were not previously recommendations on how micropollutants are given.

INTRODUCTION

Organic micropollutants (MPs) such as the active ingredients of pharmaceuticals, personal care products, and pesticides are conveyed by sanitary sewers or by surface runoff and storm sewers to wastewater treatment plants (WWTPs). There, the main removal process for polar organic MPs is microbial biotransformation in the activated sludge compartment.^{1,2} However, most MPs are not fully mineralized but rather biotransformed to transformation products (TPs), which are then released with the WWTP effluents into the aquatic environment.^{3–5} It has been shown that some TPs have the potential to be as or even more toxic than their parent MPs and thus contribute to the toxicological effects of anthropogenic chemicals on aquatic ecosystems.^{6–10} To comprehensively assess the risk of MPs, it is therefore desirable to also determine the occurrence and prevalence of their TPs in environmental water bodies. However, due to their presence at low concentrations in complex environmental matrices, the detection and identification of unknown TPs or MPs is generally challenging. Recently, screening for expected compounds in a so-called suspect screening approach has been successfully applied in different environmental matrices (e.g., wastewater effluents, lake sediments, and surface waters).^{11–15}

For the generation of a list of expected TPs for suspect screening, pathway prediction systems are helpful.^{16,17} Currently, the freely available systems for the prediction of microbial biotransformation reactions for given parent MPs include PubPred,¹⁸ CRAFT,¹⁹ the OECD toolbox,²⁰ and the EAWAG-PPS. The EAWAG-PPS derives from the former University of Minnesota pathway prediction system (UM-PPS)^{21,22} and is now hosted by Eawag, the Swiss Federal Institute of Aquatic Science and Technology.²³ The predictions of these tools are mainly based on a set of generalized biotransformation rules extracted from literature-reported, microbially mediated metabolic pathways and enzyme-catalyzed reactions. Biotransformation rules recognize functional groups present in the query compound structure and predict transformation reactions at these functional groups.²¹ Cur-

Received: October 21, 2015
 Revised: February 1, 2016
 Accepted: February 10, 2016
 Published: February 10, 2016

© 2016 American Chemical Society

DOI: 10.1021/acs.est.5b01386
 Environ. Sci. Technol. 2016, 50, 2988–2990

Everything in PDF format ☹️

Systematic storage of standardized biodegradation data



Experimental standards

- OECD (or other) guidelines
- If non-standard setups: documentation of guideline modification and/or detailed account of experimental setups is crucial



Systematic organization of data

- Pre-defined set of experimental parameters (pH, temperature, OC content, ...)
- Data-sets organized by environment (activated sludge, soil, water, ...)



Machine-readable access

- Standard formats like CSV, JSON, ...
- Database with API access (Application Programming Interface)

Schematic overview on database objects

Compounds

structure



Reactions

observed or predicted



Biotransformation rules
for reaction prediction



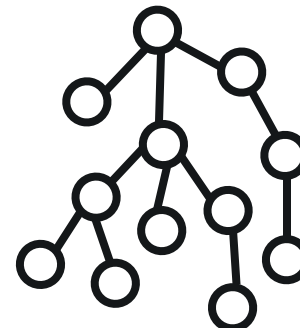
Enzymes

EC classification



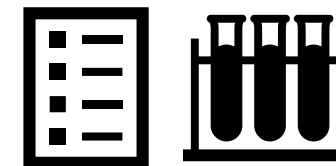
Pathways

observed or predicted



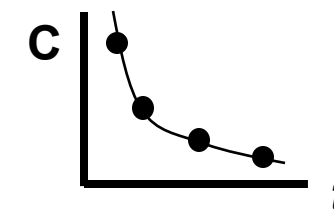
Scenarios

Experimental meta data



Biotransformation half-lives or rate constants

Obtained for specific
scenario, primary DT_{50}

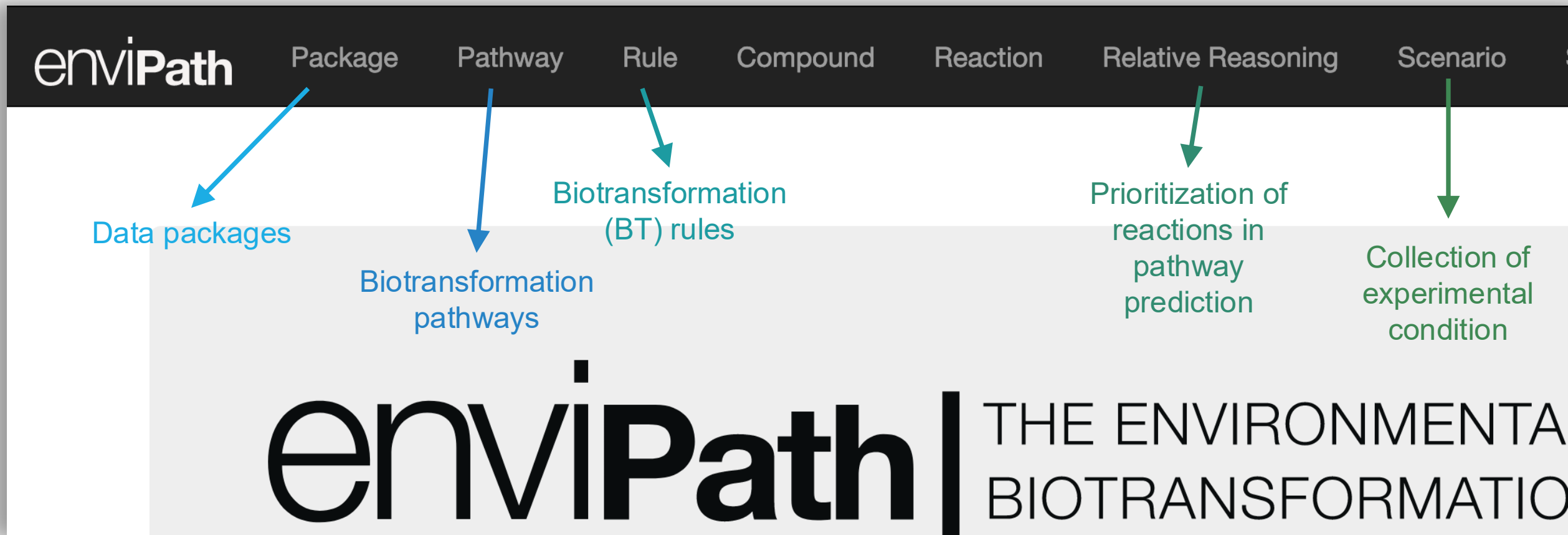




Data organization in enviPath



Overview on main objects in enviPath:

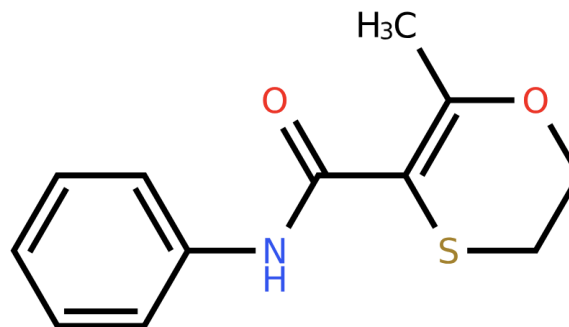


Compounds

Carboxin

Actions ▾

Image representation



SMILES representation

CC1=C(C(=O)NC2=CC=CC=C2)SCCO1

Canonical SMILES

InChIKey

Pathways

External Identifiers

Half-lives

SMILES,
canonical SMILES (without
stereochemical information),
InChIKey

Science that matters

Links to
associated
pathways,
external
database IDs
and half-lives



SMILES & SMIRKS



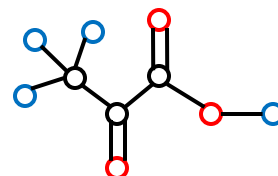
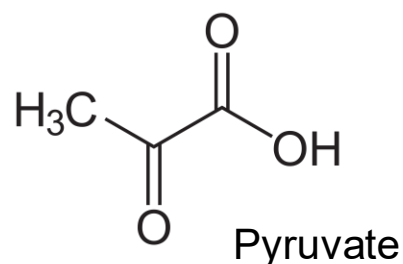
A quick introduction to cheminformatics

Graph representation

atoms = nodes

bonds = edges

Compound
SMILES

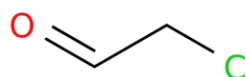
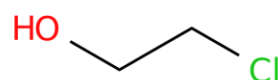


SMILES

(String representation)

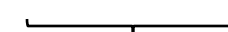
CC(=O)C(=O)O

Reaction
SMIRKS



SMIRKS

C(CO)Cl>>C(C=O)Cl


SMILES of
reactant


SMILES of
product

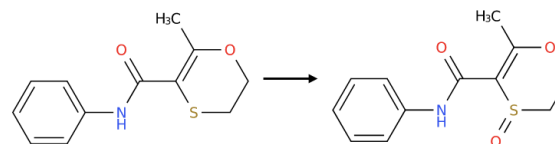
Reactions



reaction 0002303



Image representation



Reaction Description

Carboxin



P/V-16 (Carboxin sulfoxide)

SMIRKS representation

CC1=C(C(=O)NC2=CC=CC=C2)SCCO1>>CC1=C(C(=O)NC2=CC=CC=C2)S(=O)CCO1

Rules

bt0162-4180

Pathways

Biotransformation rule(s)
associated with this
reaction

Pathways

Carboxin Pathway

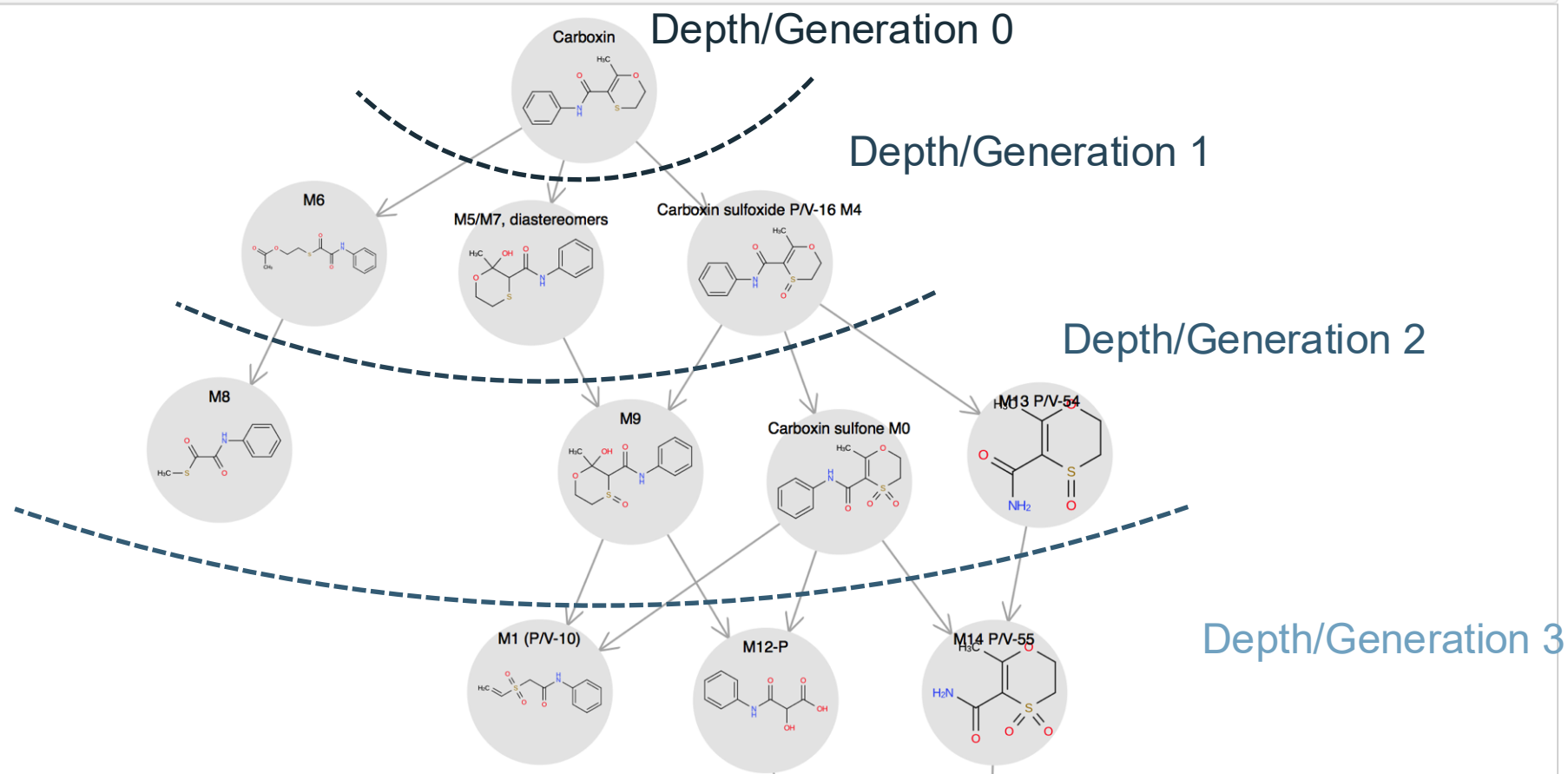
Graphical representation

Edit

View

Fullscreen

✓

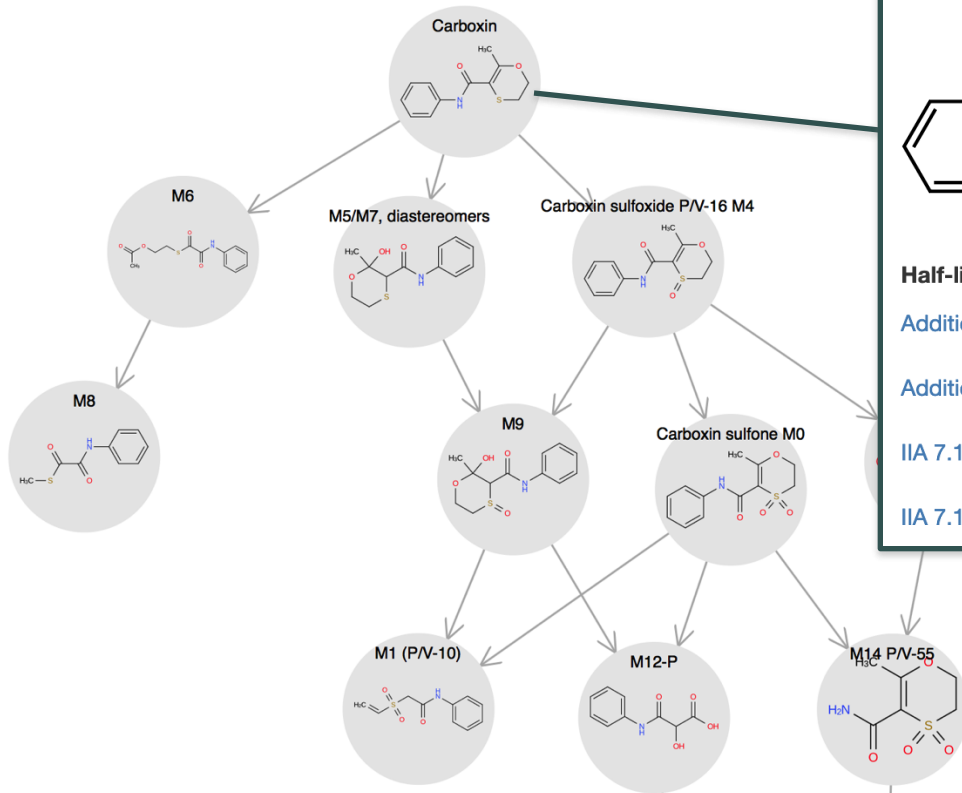


Scenarios

Carboxin Pathway

Graphical representation

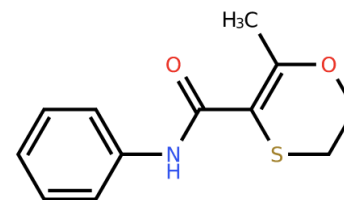
Edit View



Compound

Carboxin

Depth: 0



Half-lives and related scenarios:

[Additional report, IIA 7.1.1.1.1/06, Mamouni, 2007 - \(00000\) \(Related Scenario\) - \(00000\)](#)

[Additional report, IIA 7.1.1.1.1/06, Mamouni, 2007 - \(00001\) \(Related Scenario\) - \(00000\)](#)

[IIA 7.1.1.1.1/01, Mamouni, 2004, 7.1.1.2.1/01, Wanner, 2004b - \(00000\) \(Related Scenario\) - \(00000\)](#)

[IIA 7.1.1.1.1/01, Mamouni, 2004, 7.1.1.2.1/01, Wanner, 2004b - \(00001\) \(Related Scenario\) - \(00000\)](#)

Home / Package / EAWAG-SOIL - Scenario / IIA 7.1.1.1.1/03, Dzialo, 1989a - (00000) (Related Scenario) - (00000)		
IIA 7.1.1.1.1/03, Dzialo, 1989a - (00000) (Related Scenario) - (00000) ★		
Property	Value	Unit
Acidity	Value: 6.8 Measurement Methods:	pH
Cation exchange capacity, CEC	6.9	mEq/100g
Half-life	DT50: 1.06 Model: SFO Fit: reported non-linear regression used by rapporteur Source: IIA 7.1.1.1.1/03, Dzialo, 1989a	d
Organic content	2.73	OC
Redox condition	aerobic	
Soil texture	Sandy loam Sand: 63.0% Silt: 31.0% Clay: 6.0%	
Soil texture classification system	USDA	
Spike compound	Spike compound 0000318 	
Spike concentration	2.9	µg/kg dry soil

Scenario

Contains:

- Experimental conditions
- Half-lives (DT₅₀s)

Biotransformation rules

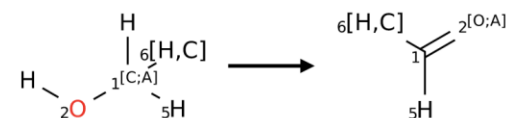
bt0001-3568



Description

primary Alcohol > Aldehyde

Representation



Reaction

SMIRKS

[H][#8:2][C:1]([H:5])([H])(#1,#6:6)>>[H:5][#6:1](-[#1,#6:6])=[O:2]

Reactants Smarts

Products Smarts

Included in Composite-Rule

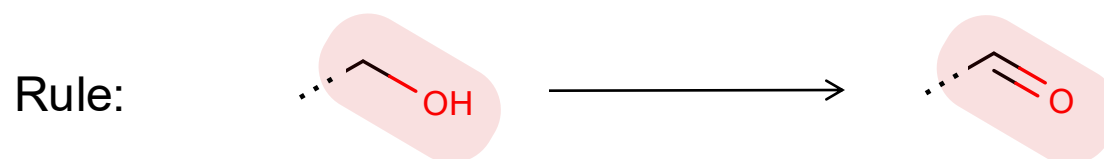
Reactant Filter Smarts

Scenarios

Reactions

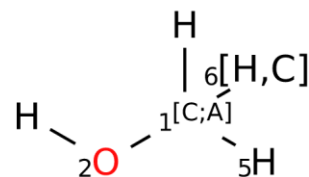
Pathways

Biotransformation rules



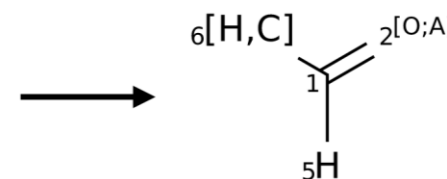
Recognition

Find -OH group on molecule



Transformation

Rearrange bonds to get =O group



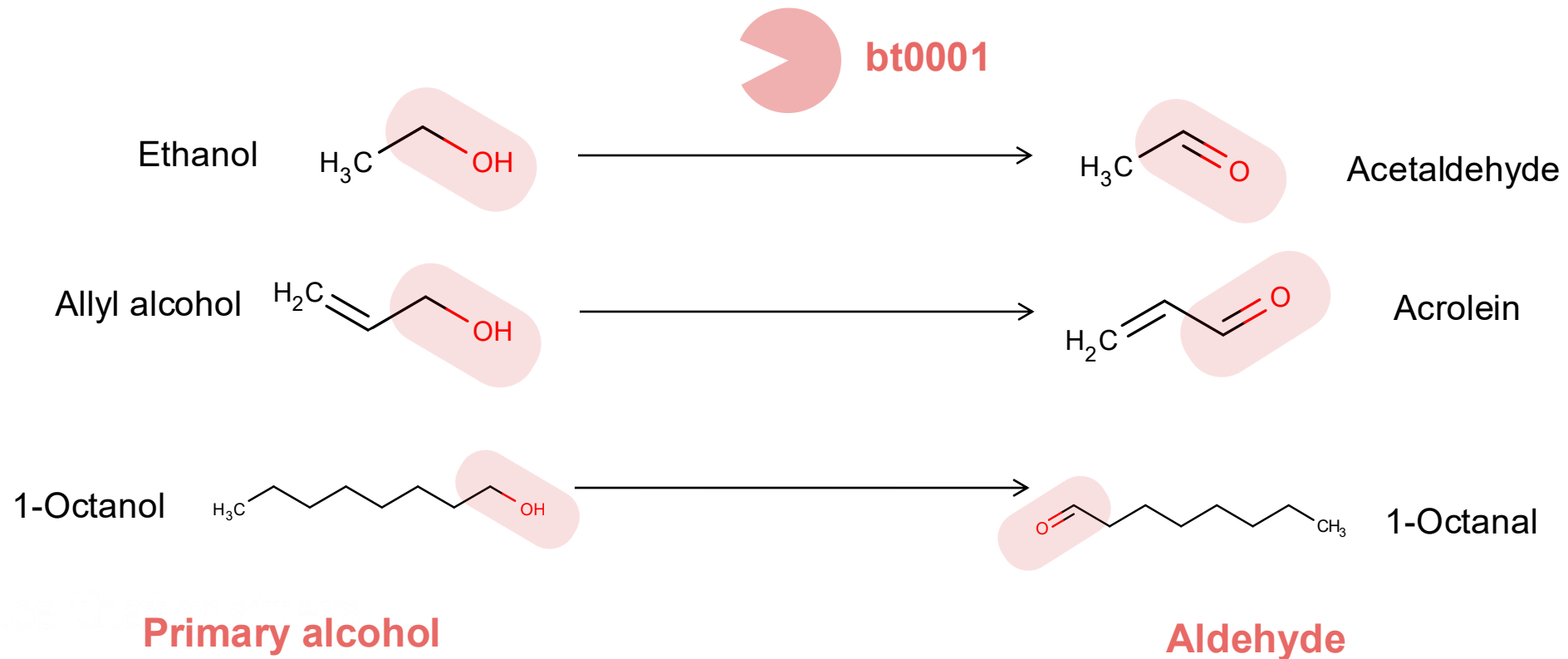
SMARTS

[H][#8:2][C:1]([H:5])([H])[#1,#6:6]

[H:5][#6:1](-[#1,#6:6])=[O:2]

Biotransformation rules

Example: Substrate-promiscuous action of an alcohol dehydrogenase



Biotransformation (BT) rules in enviPath

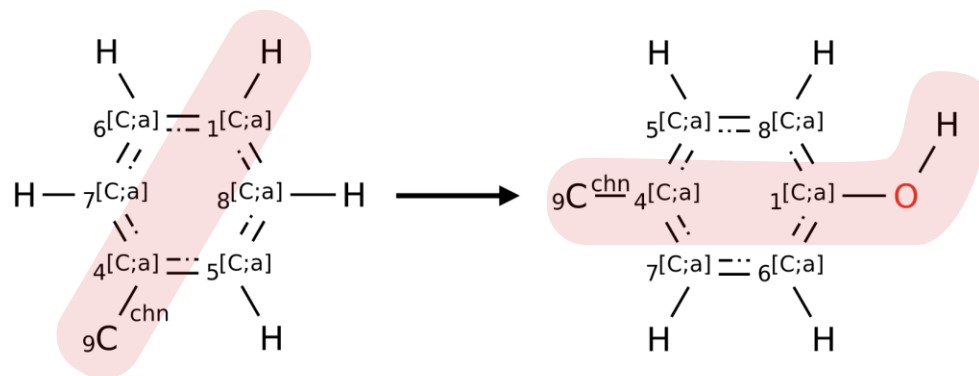


499 expert-curated biotransformation rules

- Rule names start with bt....
- They can consist of several sub-rules (“parallel rules”), for example bt0013:

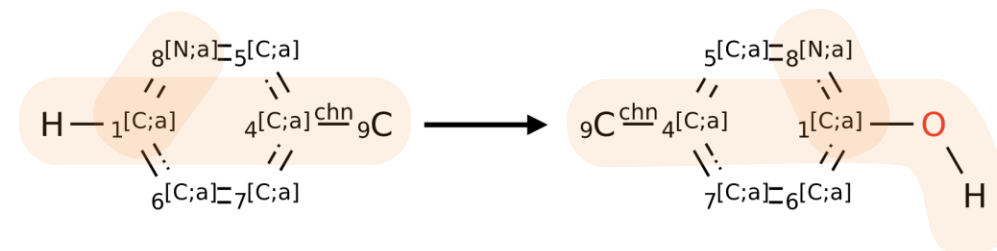
bt0013-4165

monosubstituted Benzenoid → Add p-OH







bt0013-4165.2

substituted Pyridine → Add p-OH



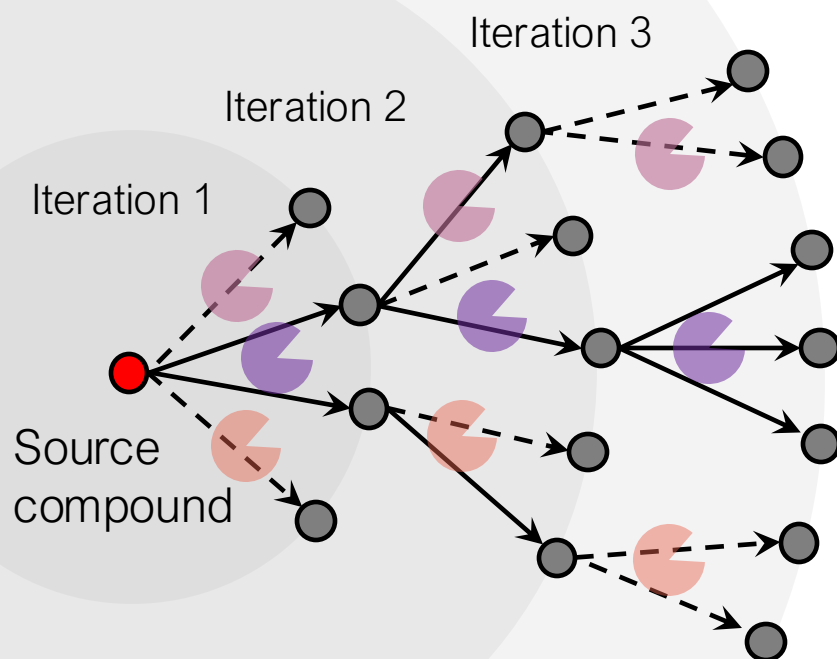
Rules linked to EC classification (enviLink)

Example: bt0001

EC Numbers			
1.1.1.-			
1.1.1.1	alcohol dehydrogenase	enviPath	EAWAG-BBD 2020-10-21 enviLink
1.1.1.1	alcohol dehydrogenase		KEGG 2020-10-21 enviLink
1.1.1.2	alcohol dehydrogenase (NADP+)		KEGG 2020-10-21 enviLink
...			
1.1.2.-		enviPath	
1.1.2.7	methanol dehydrogenase	enviPath	EAWAG-BBD 2020-10-21 enviLink
1.1.3.-			
1.1.3.7	aryl-alcohol oxidase		KEGG 2020-10-21 enviLink
1.1.3.9	galactose oxidase		KEGG 2020-10-21 enviLink
...			

From reaction to pathway prediction

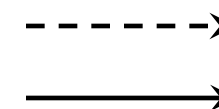
Degradation pathway prediction through iterative rule application



1. **biotransformation rules**,
expert-curated, 499 rules



2. **Relative reasoning rules**:
Prioritization of
biotransformation reactions



→ **More on this later today!**

2. Data packages in enviPath

Available data packages

EAWAG-BBD

Data obtained from **original UMBBD**

Pathways observed mostly in **pure or enrichment cultures**

Pathways	✓
Compounds	✓
Reactions	✓
BT rules	✓
Scenarios	✗
Enzymes	✓



EAWAG-SOIL, EAWAG-SLUDGE, EAWAG-SEDIMENT

Data obtained from **literature** and **regulatory reports**

Pathways and half-lives observed in **complex natural or technical (WWTP) cultures**

Pathways	✓
Compounds	✓
Reactions	✓
BT rules	(✓)
Scenarios	✓
Enzymes	✗



EAWAG-BBD: Heritage from UM-BBD/PPS

Data in EAWAG-BBD

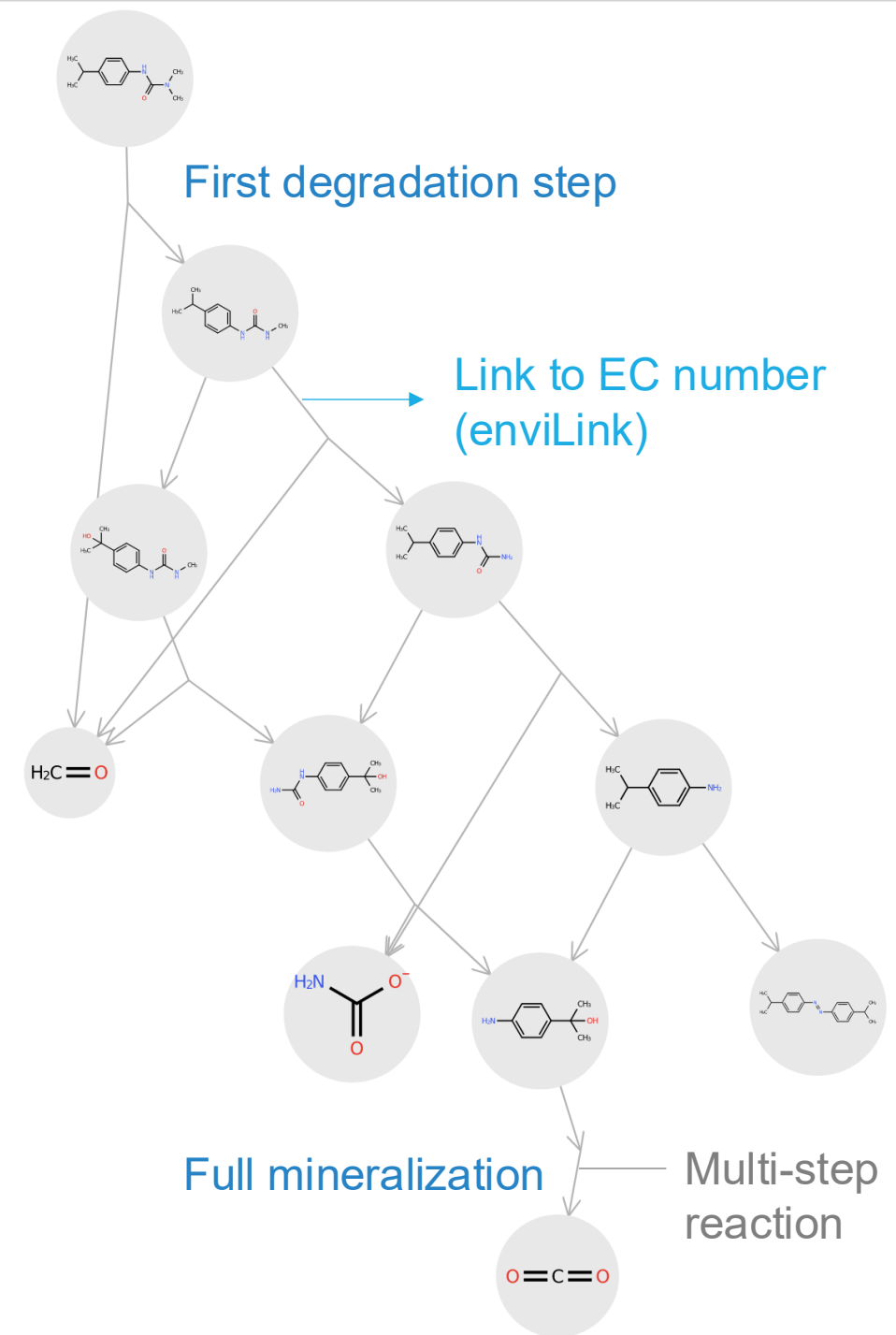
EAWAG-BBD	
Experimental guideline	None - pathways obtained mostly from pure and enrichment cultures
Type of chemicals	Diverse - Industrial chemicals, pesticides, pharmaceuticals, natural products
Source	Scientific literature (publication date ranging from 1957 to 2011)
# Pathways	220
# Compounds	648
# Reactions	1480 (associated with ~ 900 enzymes)
# BT rules	499

Example: Isoproturon pathway

Available information: Compilation of 4 studies

Description

The phenylurea herbicide isoproturon (IPU) is used against annual grasses and broad-leaved weeds in cereal production across Europe, resulting in both surface water and ground water pollution (Sorensen et al., 2001). Isoproturon in soil is degraded, producing carbon dioxide and degradation products (Perrin-Ganier et al., 2001). The major biodegradation pathway of isoproturon is isoproturon → mono-demethyl-isoproturon → hydroxy-monodemethyl-isoproturon → 4'-(2-hydroxyisopropylphenyl)urea → 4'-(2-hydroxyisopropylphenyl)aniline. Other minor pathways exist. Through one of these, 4,4'-diisopropylazobenzene can accumulate in soil (Perrin-Ganier et al., 2001). Attempts to isolate microorganisms which metabolize isoproturon have often failed. Recently, Sphingomonas sp. strain SRS2 was found to mineralize isoproturon. Sphingomonas sp. strain SRS2 is auxotrophic; it requires strain SRS1 to supply amino acids needed for the pathway (Sorensen et al., 2002).



Available data packages

EAWAG-BBD

Data obtained from **original UMBBD**

Pathways observed mostly in **pure or enrichment cultures**

Pathways	✓
Compounds	✓
Reactions	✓
BT rules	✓
Scenarios	✗
Enzymes	✓



EAWAG-SOIL, EAWAG-SLUDGE, EAWAG-SEDIMENT

Data obtained from **literature** and **regulatory reports**

Pathways and half-lives observed in **complex natural or technical (WWTP) cultures**

Pathways	✓
Compounds	✓
Reactions	✓
BT rules	(✓)
Scenarios	✓
Enzymes	✗



Data collections in envPath

3 environment-specific data packages

enviPath

	EAWAG-SOIL	EAWAG-SLUDGE	EAWAG-SEDIMENT
Guideline	OECD 307	N/A	OECD 308
Type of chemicals	Pesticides	Micropollutants in general	Pesticides
Source	Regulatory reports	Scientific literature	Regulatory reports
# Pathways	317	183	179
# Compounds	1780	1067	579
# Cpds with half-lives	895	158	181
Status	Published (2017)	Published (2023)	Published (2025)



Data in EAWAG-SOIL



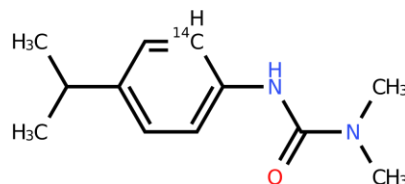
Biodegradation experiments in soil

Guideline: OECD 307



¹⁴C-labeled spike compound

- Structure
- Spike concentration



Experimental conditions

- Temperature
- pH
- Redox condition

Experimental outcome

- **Half-life**
 - determined from concentration-time series
 - Model used for HL determination, model fit, comments
- **Transformation products**
 - Structure
 - % radioactivity (major/minor classification)



Soil parameters

- Soil texture (% sand, silt, clay)
- Organic carbon content
- Cation exchange capacity (CEC)
- Water storage capacity



EAWAG-SOIL

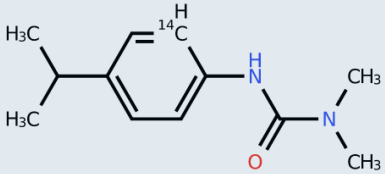
Scenario

Spike compound

Experimental conditions

Soil parameters

Experimental outcome

Property	Value	Unit
Acidity	Value: 6.8 Measurement Methods:	pH
Cation exchange capacity, CEC	12.5	mEq/100g
Half-life	DT50: 10.9 Model: SFO Fit: Comment: Source: Galicia (1989); Callow & Jarvis (2011)	d
Organic content	1.3	OC
Redox condition	aerobic	
Soil origin	SLH	
Soil texture	Silt loam Sand: 14.8% Silt: 65.5% Clay: 19.7%	
Spike compound	Spike compound 0000381 	
Spike concentration	2.0	µg/kg dry soil
Temperature	20.0	°C
Water storage capacity	water hold capacity 13.4 conditions % actual WC maximum water hold capacity	g water/100g dry soil

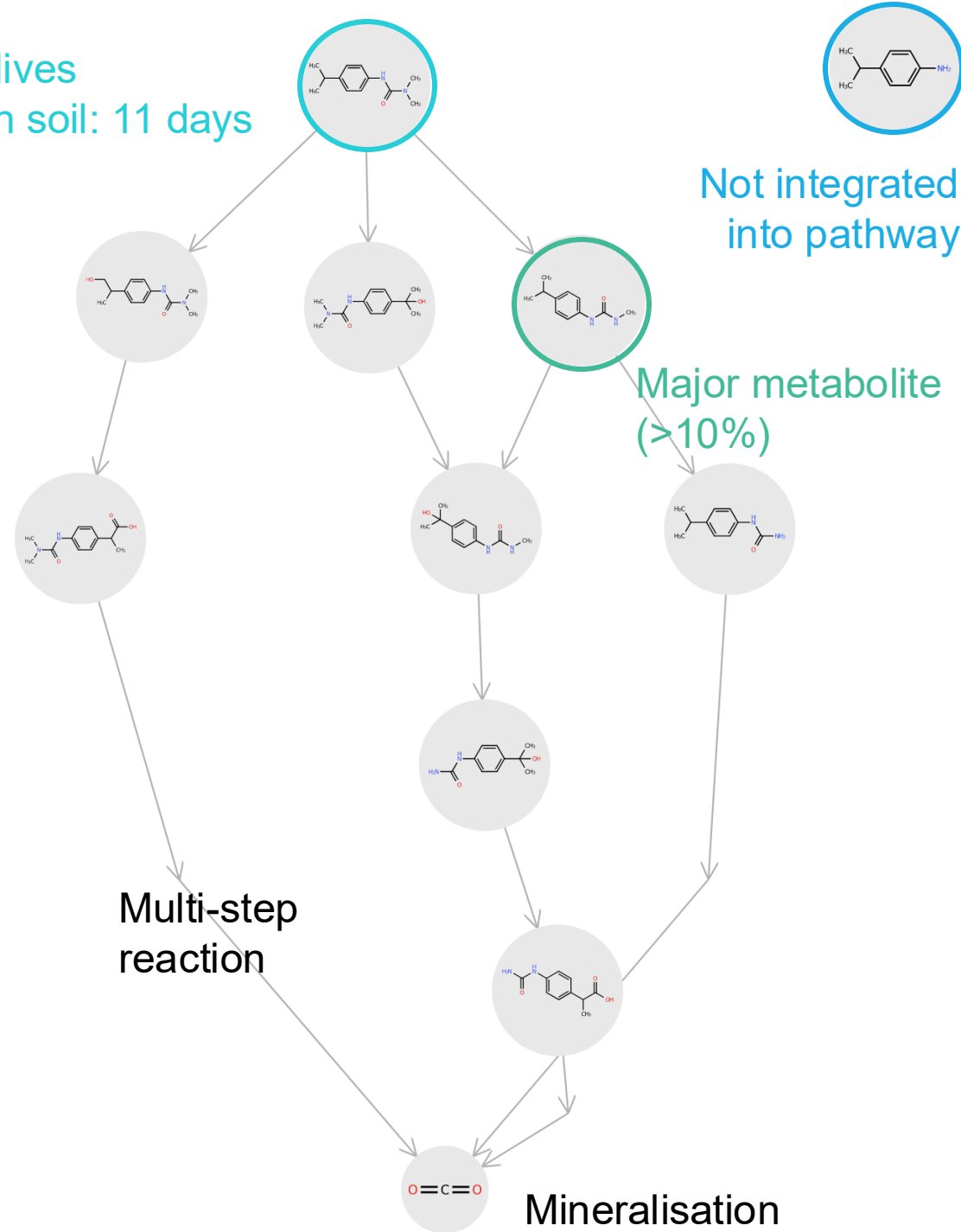
- 14 reported half-lives
- Median half-life in soil: 11 days

Example: Isoproturon pathway

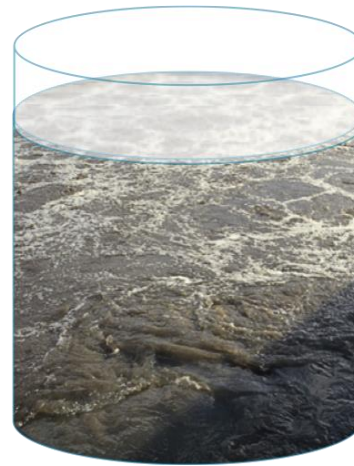
Compilation of several studies

Description

Aerobic degradation studies in soil demonstrated that isoproturon was degraded via biological processes, with 10 to 45% mineralisation after 58 to 100 days and unextractable residues of 48 to 73% of applied radioactivity after 58 to 100 days. In the Review Report for isoproturon (SANCO/3045/99-final 12 March 2002), only the metabolite desmethyl-isoproturon was classified as a major metabolite (occurring in amounts >10% of applied substance). [...] The degradation pathway of isoproturon involves demethylation (to produce desmethyl-isoproturon) and hydroxylation (to produce 1-OH-isoproturon and 2-OH-isoproturon) forming three primary metabolites (which were identified as potentially relevant). Desmethyl-isoproturon is transformed to didesmethyl-isoproturon in a second demethylation step. 1-OH-isoproturon degrades further to proanoic acid isoproturon, whereas 2-OH-isoproturon is transformed to minor metabolites.



Data in EAWAG-SLUDGE



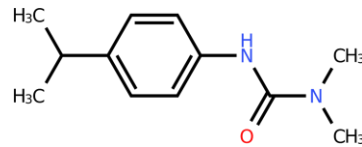
Biodegradation experiments in activated sludge

(OECD 314b)



Spike compound (unlabeled)

- Structure
- Spike concentration
- Type of compound addition



Experimental outcome

- **Rate constant or half-life**
 - determined from concentration-time series
 - Model used for HL determination, model fit, comments
- **Transformation products**
 - Structure
 - Confidence level

Experimental conditions

- Temperature
- pH
- Redox condition

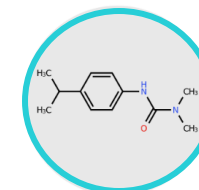
Sludge parameters

- Setup
 - Bioreactor type
 - Aeration
- Origin
 - Location
 - Treatment technology
- Sludge properties
 - N, P content
 - Total suspended solids concentration (TSS)

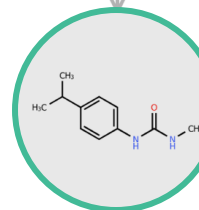


Example: Isoproturon pathway

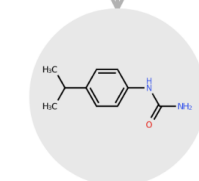
Compilation of several studies



- 14 reported rate constants or half-lives
- Median half-life in sludge: 6.8 days

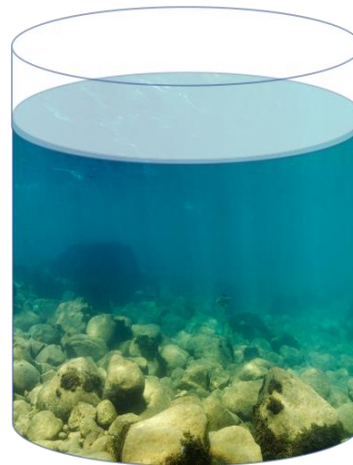


Sometimes
Level of confidence for
metabolite identification*



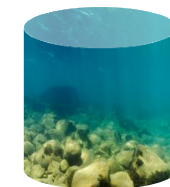
* According to Schymanski *et al. Environ. Sci. Technol.* **48**, 2097–2098 (2014).

Data in EAWAG-SEDIMENT



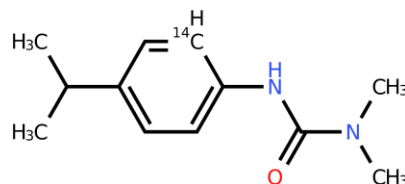
Biodegradation experiments in water-sediment systems

Guideline: OECD 308



¹⁴C-labeled spike compound

- Structure
- Spike concentration

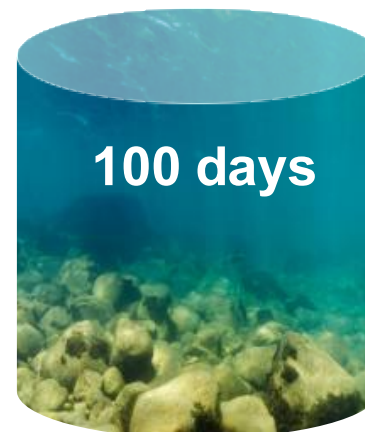


Experimental conditions

- Temperature
- pH (water and sediment)
- Redox potential
- Oxygen content

Experimental outcome

- **Half-lives** (total system, water, sediment)
 - determined from concentration-time series
 - Model used for HL determination, model fit, comments
- **Transformation products**
 - Structure
 - % radioactivity (major/minor classification)



Water-sediment parameters

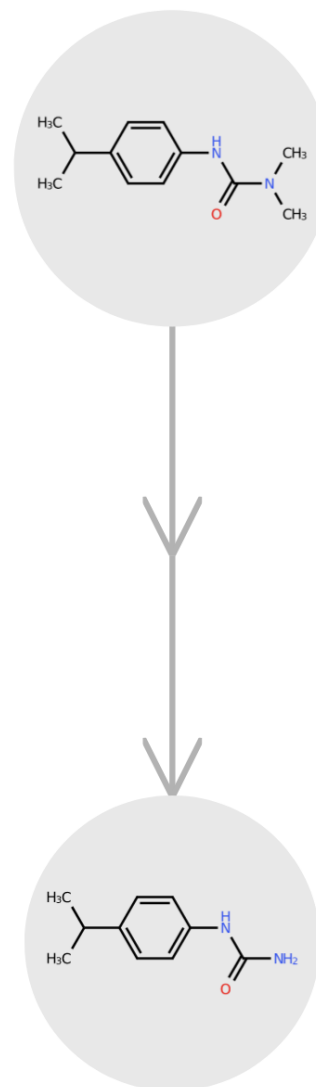
- Sample location
- Sediment texture
- Ratio water to sediment
- Organic content
- Sediment porosity

Example: Isoproturon pathway

One study in a water-sediment system

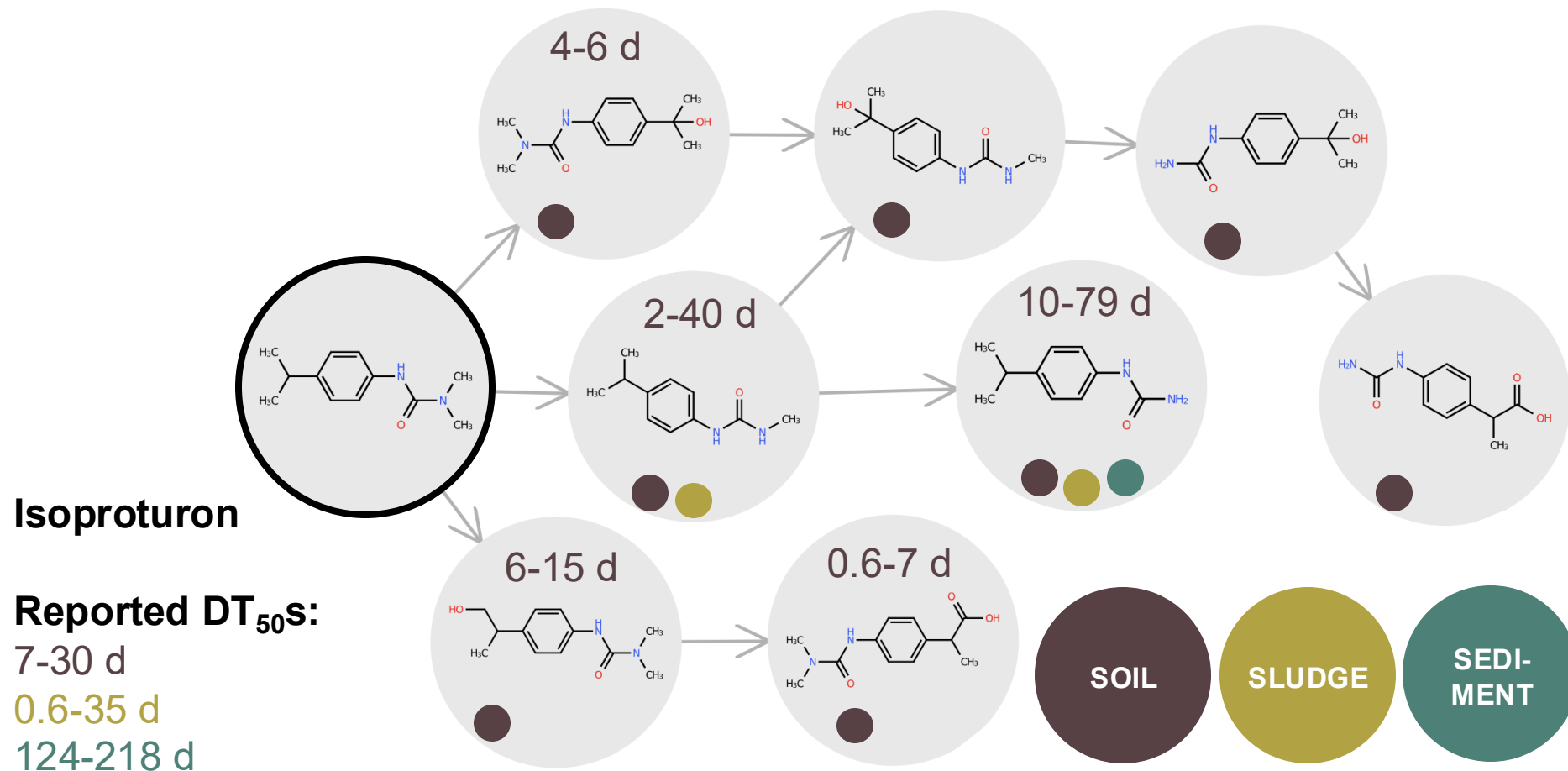
Description

The route and rate of degradation of ¹⁴C-isoproturon in two aquatic systems (Bury Pond: fine texture, Emperor Lake: coarse texture) under aerobic conditions were investigated at 20 °C in the dark. In the entire system the half-lives of ¹⁴C-isoproturon were calculated to be 101 and 279 days for pond and lake systems. Two metabolites exceed the 5 or 10 % AR in water or sediment: Desmethyl-isoproturon (whole system: 20.9%) and BPh1 (whole system: 9.5%).



→ Systematic comparison between packages ?

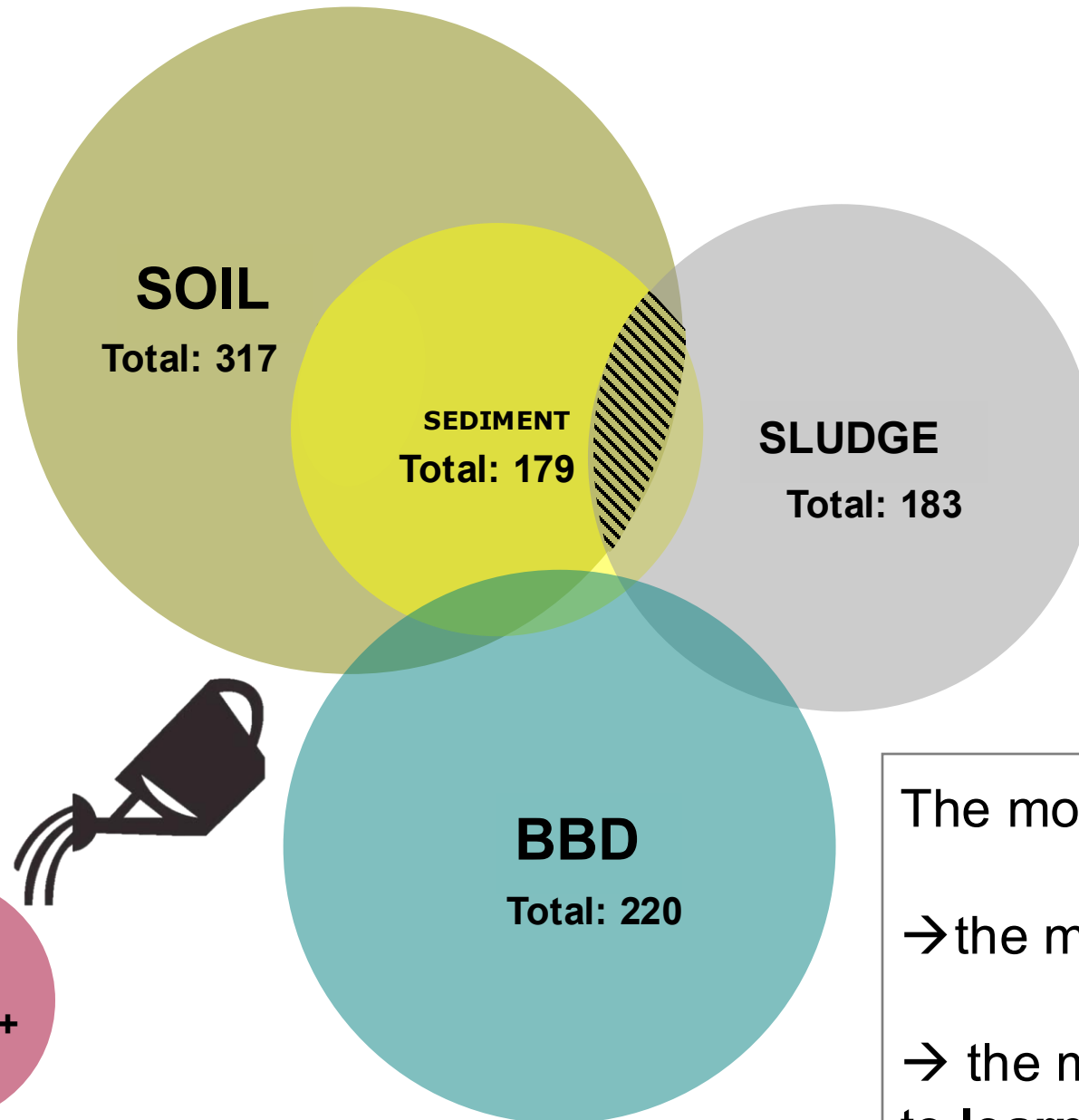
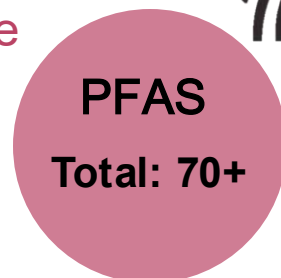
Comparison of Isoproturon pathways



Overlap between BBD, SOIL, SLUDGE, and SEDIMENT

Common pathways

Talk by Stephanie
in the afternoon



The more **data**

→ the more **overlap**

→ the more opportunities
to **learn** from data

SOIL vs. SLUDGE vs. SEDIMENT

Comparing data packages – opportunities for read-across

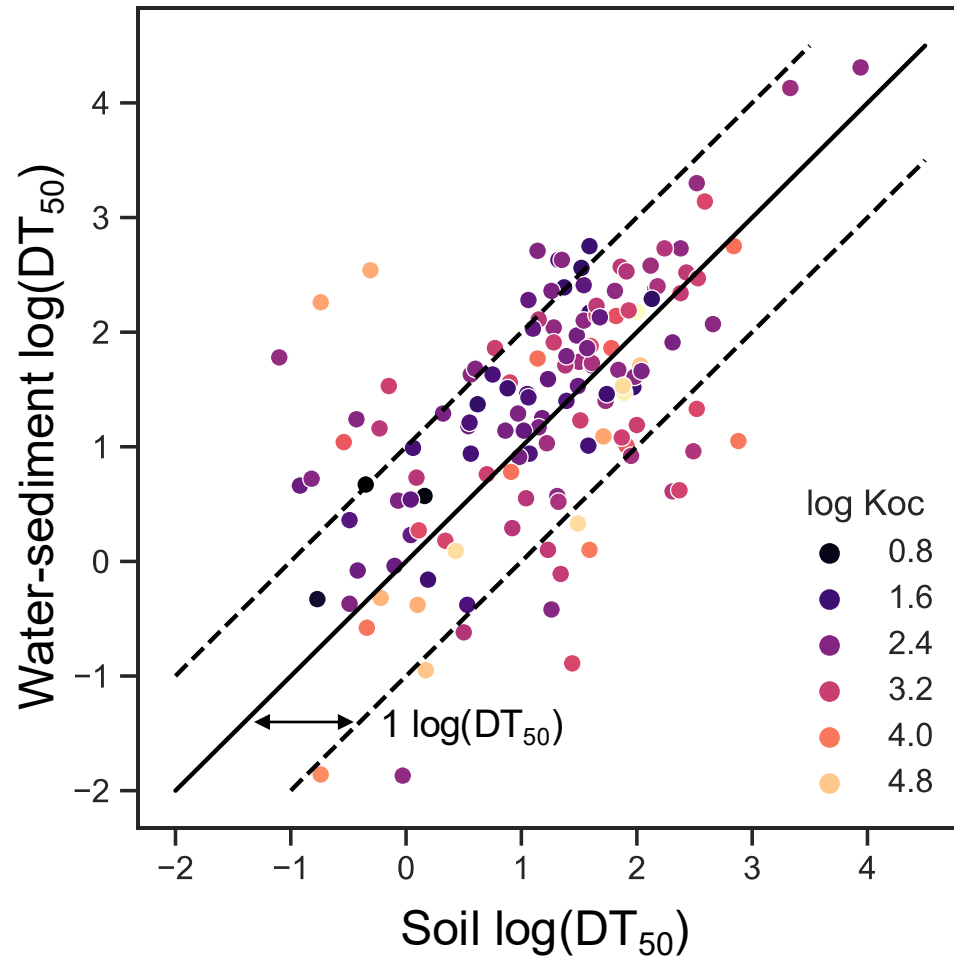
8 common pathways*	SOIL	SLUDGE	SEDIMENT
Average number of TPs	6.6	2.3	1.1
Average half-lives	12 days	3 days	52 days

→ Shortest **half-lives** in activated sludge, longest in water-sediment systems

→ Most **transformation products** detected in soil, very few in sediment

* Carbetamide, Clomazone, Diazinon, Ethofumesate, Isoproturon, Napropamide, Spiroxamine, Trinexapac-ethyl

SOIL vs. SEDIMENT half-lives



Information

148 Pesticides and pesticide TPs

logDT50 values: Bayesian mean, in log(days)

logK_{oc} values predicted by OPERA

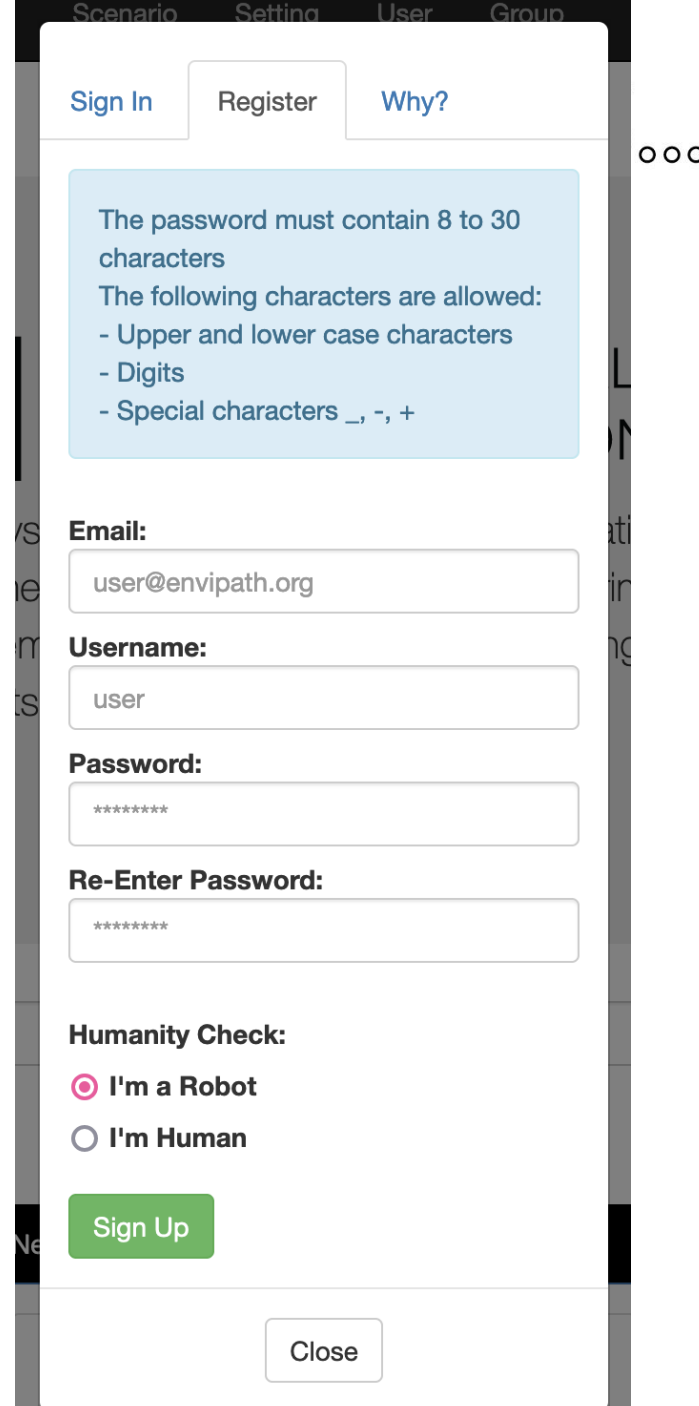
3. Navigating enviPath data

User administration

Users can ...

- register and create own packages
- establish groups
- give reading and writing rights for their packages
- submit packages for review and publication on enviPath
- Define default settings for their package

How to register →



The screenshot shows a registration modal window with the following elements:

- Navigation tabs:** Sign In, Register (active), Why?
- Password requirements (blue box):**
 - The password must contain 8 to 30 characters
 - The following characters are allowed:
 - Upper and lower case characters
 - Digits
 - Special characters `_`, `-`, `+`
- Email:** user@envipath.org
- Username:** user
- Password:** masked with asterisks
- Re-Enter Password:** masked with asterisks
- Humanity Check:**
 - ☒ I'm a Robot
 - ☐ I'm Human
- Sign Up:** A green button to submit the registration.
- Close:** A button at the bottom right to dismiss the modal.

enviPath Python API

API: Application Programming interface

Freely available at <https://github.com/enviPath/enviPath-python>

Tutorials can be found here: <https://envipath-python.readthedocs.io>

```
# Define the instance to use
INSTANCE_HOST = 'https://envipath.org'
# Each journey starts with setting up the enviPath instance
eP = enviPath(INSTANCE_HOST)
# Define package URIs
BBD_URI = 'http://envipath.org/package/32de3cf4-e3e6-4168-956e-32fa5ddb0ce1'
# Load package BBD
bbd = Package(eP.requester, id=BBD_URI)
# Retrieve data from enviPath
bbd_compounds = bbd.get_compounds()
bbd_pathways = bbd.get_pathways()
```

Take-home message

- ✓ envPath is a growing **resource** for biodegradation data
- ✓ The data can be used to develop predictive **models** (TPs, half-lives)
- ✓ Maybe **YOU can contribute** to expand our knowledge base in the future !

Acknowledgements

enviPath team

Prof. Kathrin Fenner

Tim Lorsbach

Dr. Jörg Wicker

Kunyang Zhang

Athira Shankar

Albert Anguera Sempere

Data upload & curation

Stephanie Rich

Moritz Salz

Christoph Leu

Tseng-Wei Lee

Ananya Manchanda

Data production (experiments)

Leo Trostel

Dr. Claudia Coll

Funding sources



European
Commission

Horizon 2020
European Union funding
for Research & Innovation

swissuniversities