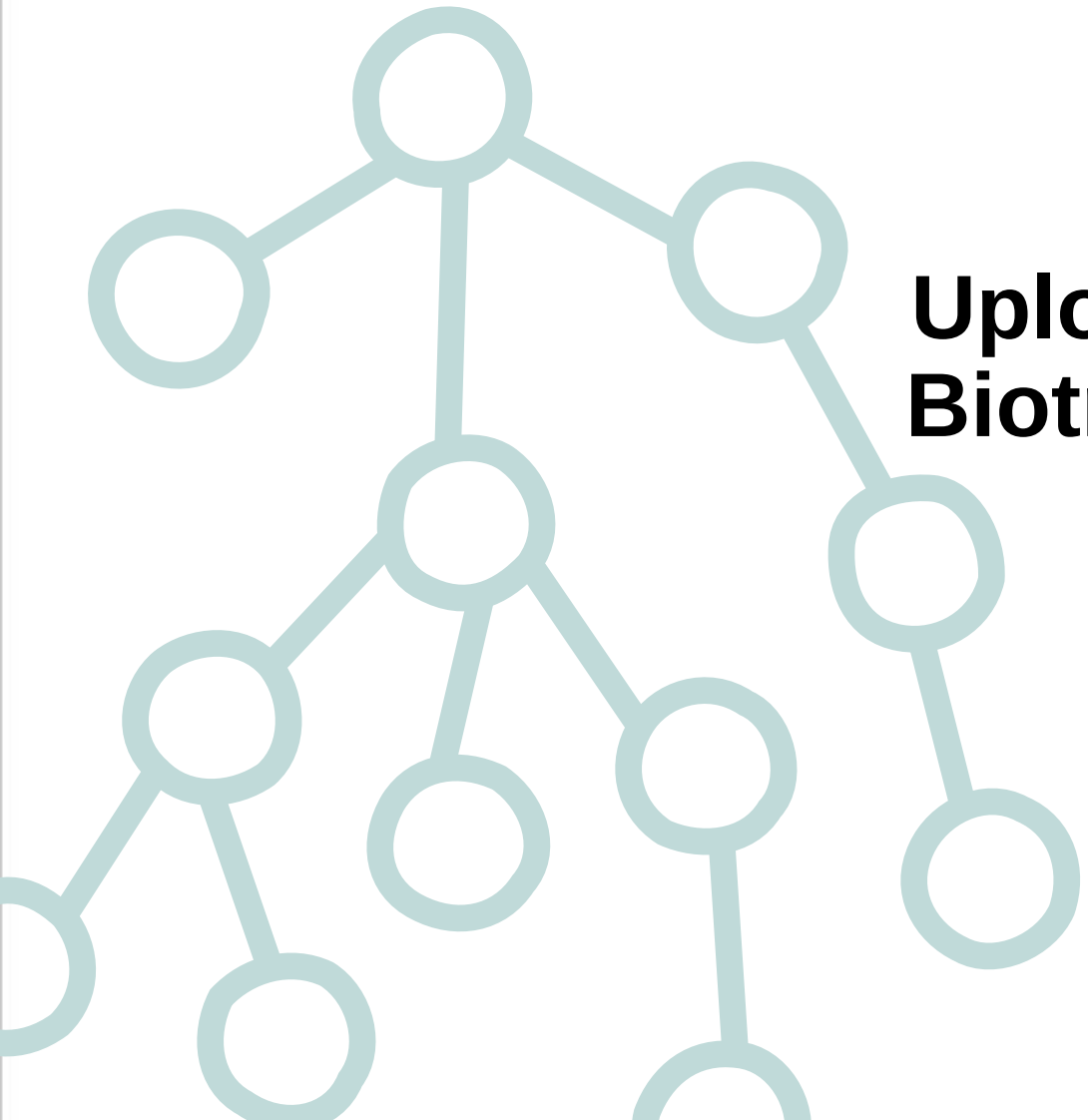
Universität Zürich[UZH]

Eawag
Swiss Federal Institute of Aquatic Science and Technology

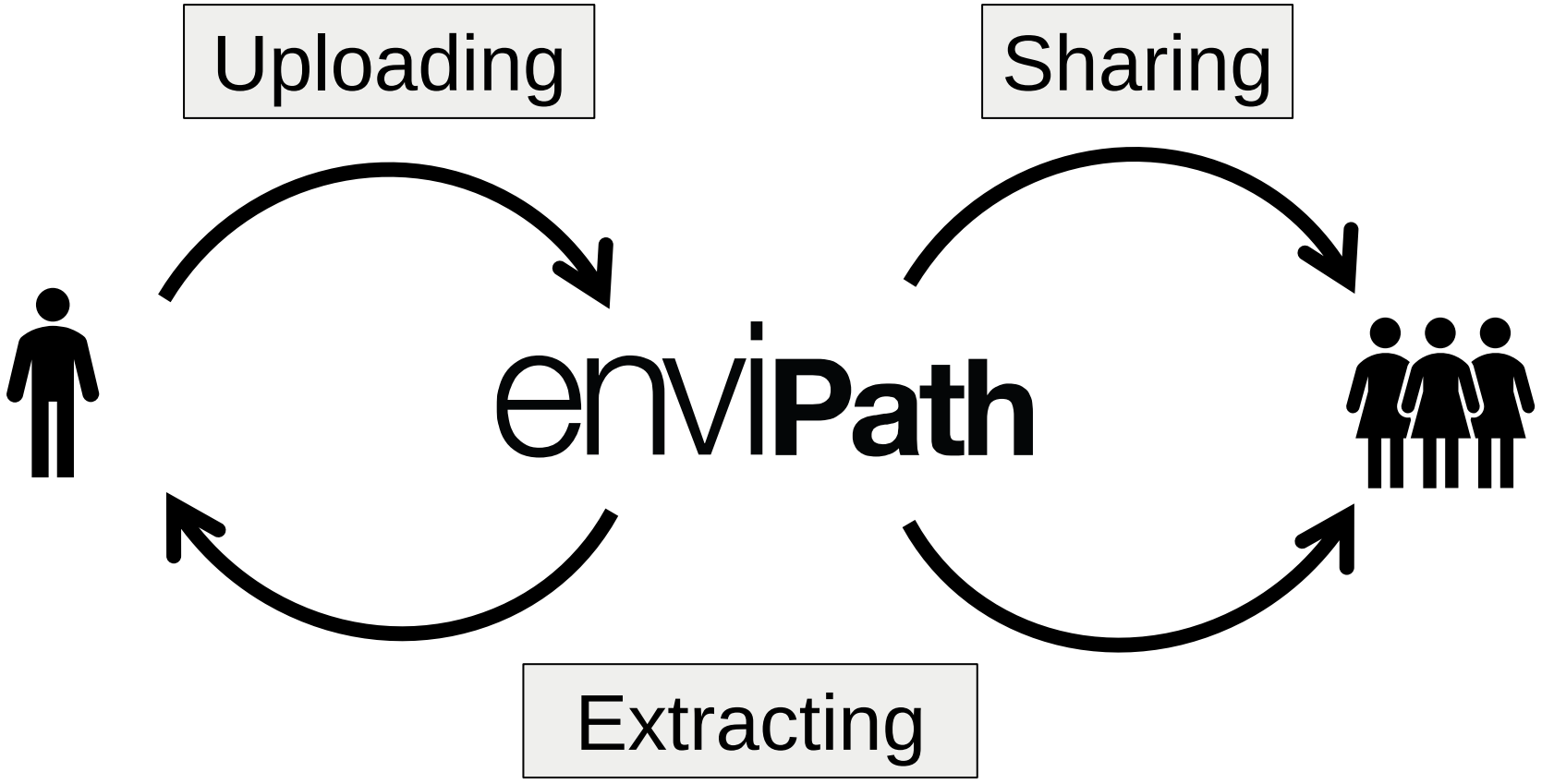
eawag aquatic research



Uploading, Sharing, and Extracting Biotransformation Data in enviPath

May 11th 2025

Synthesizing data on environmental contaminant biotransformations requires community-driven efforts



Literature Review

Trend Analysis

Model Building

There are two ways you can upload your data to enviPath

My publication

Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat.

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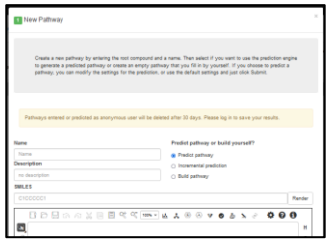
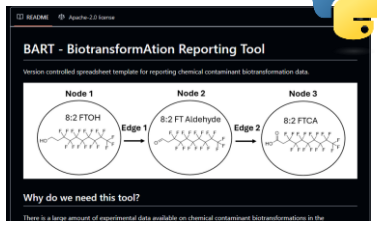
The enviPath Website



The Biotransformation Reporting Tool



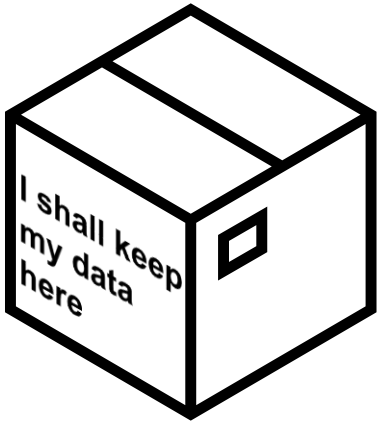
Database

Biodegradation data – pathways, half-lives, experimental conditions

The enviPath website – good for uploading small datasets

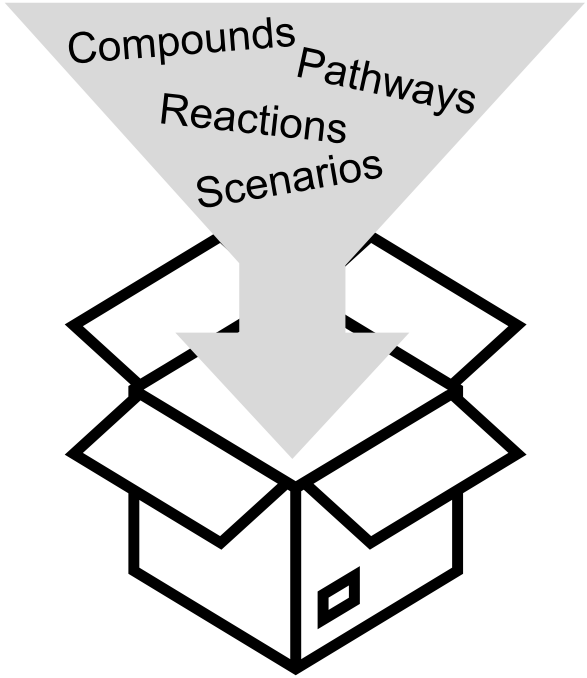
1

Create an empty package



2

Add your data to the empty package



3

Make package public

Where does your data come from?

"We built our random-forest model using the enviPath-PFAS package in addition to our own experimental data"

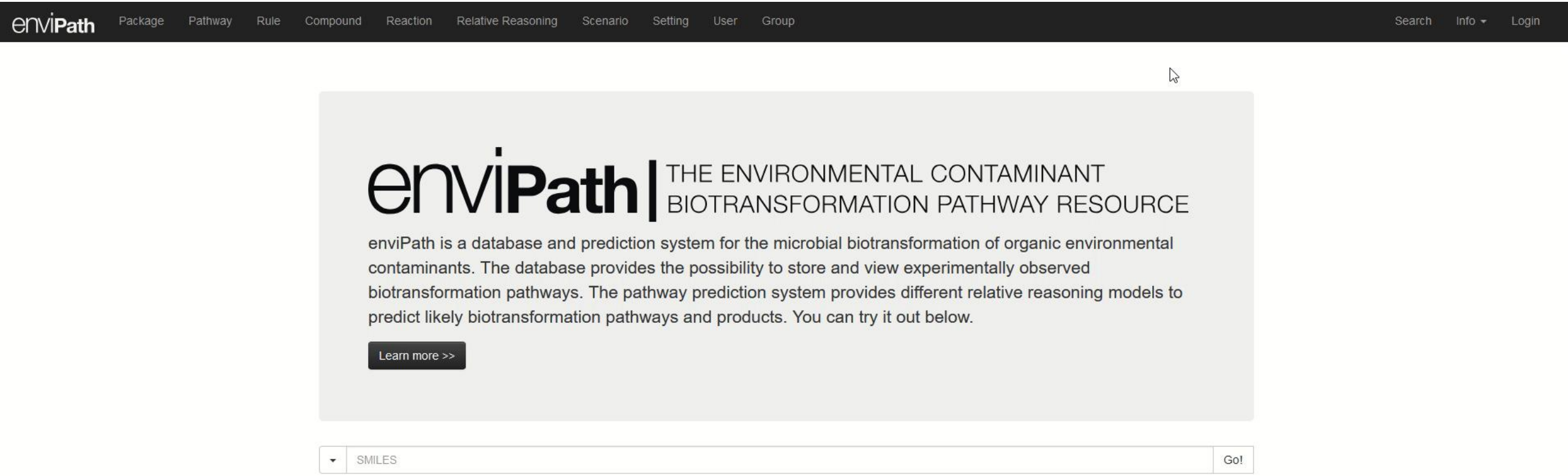
We require you to publish your data in a FAIR format

"Our dataset is publicly available on the enviPath platform"

Getting started with the enviPath website

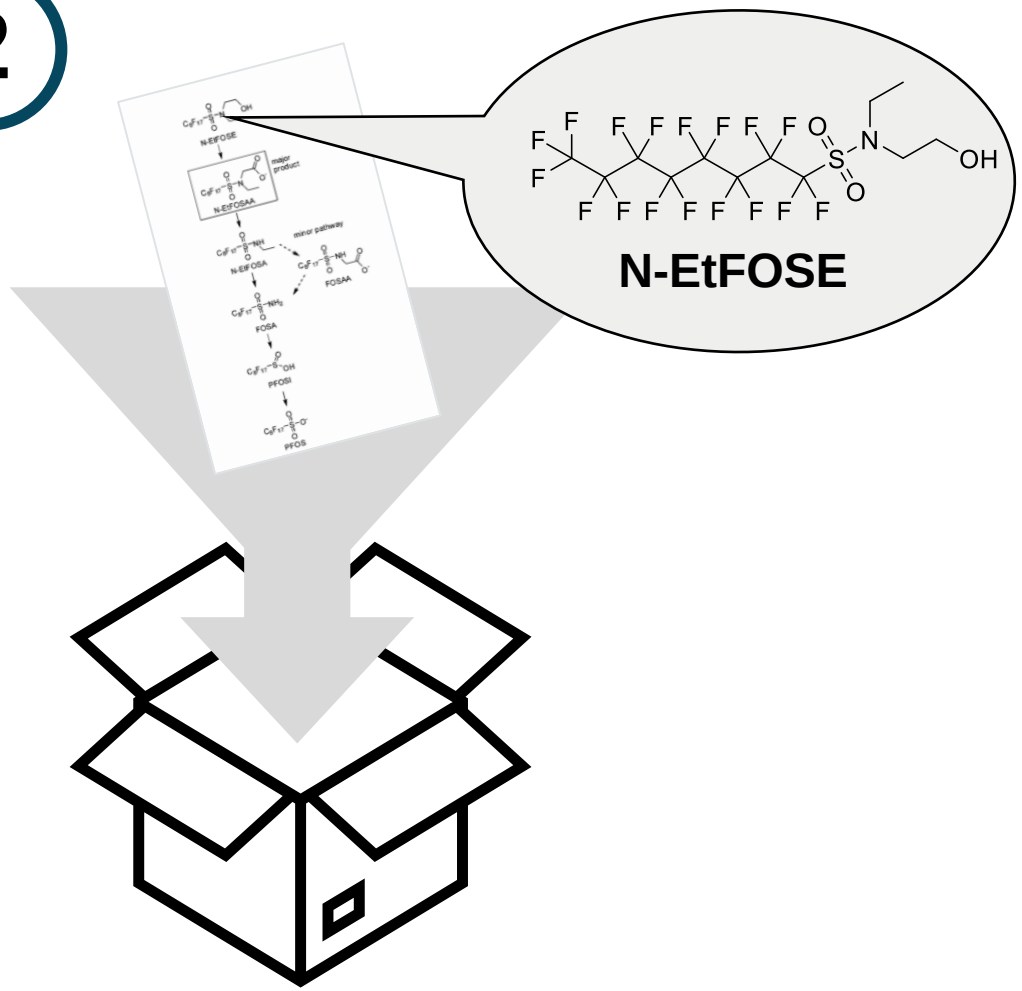
1

Sign in to enviPath → Create an empty package



Add a pathway starting with the parent compound

2



Home / Package / Test Package 1

Test Package 1 — Actions

Test package for SETAC Workshop

Pathways	0
Rules	0
Compounds	0
Reactions	0
Relative Reasoning	0
Scenarios	0

eawag aquatic research

THE UNIVERSITY OF AUCKLAND NEW ZEALAND | SCIENCE SCHOOL OF COMPUTER SCIENCE MACHINE LEARNING

Contact

enviPath UG (haftungsbeschränkt

Add transformation products (TPs) to the pathway

2

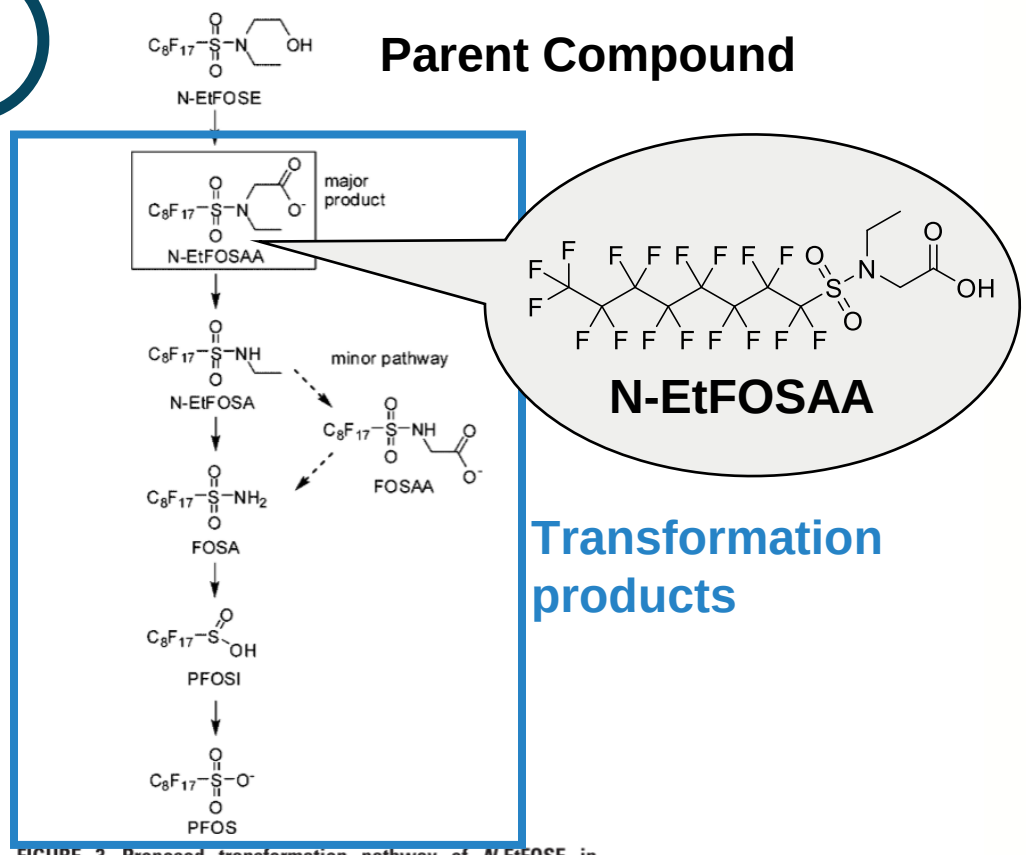
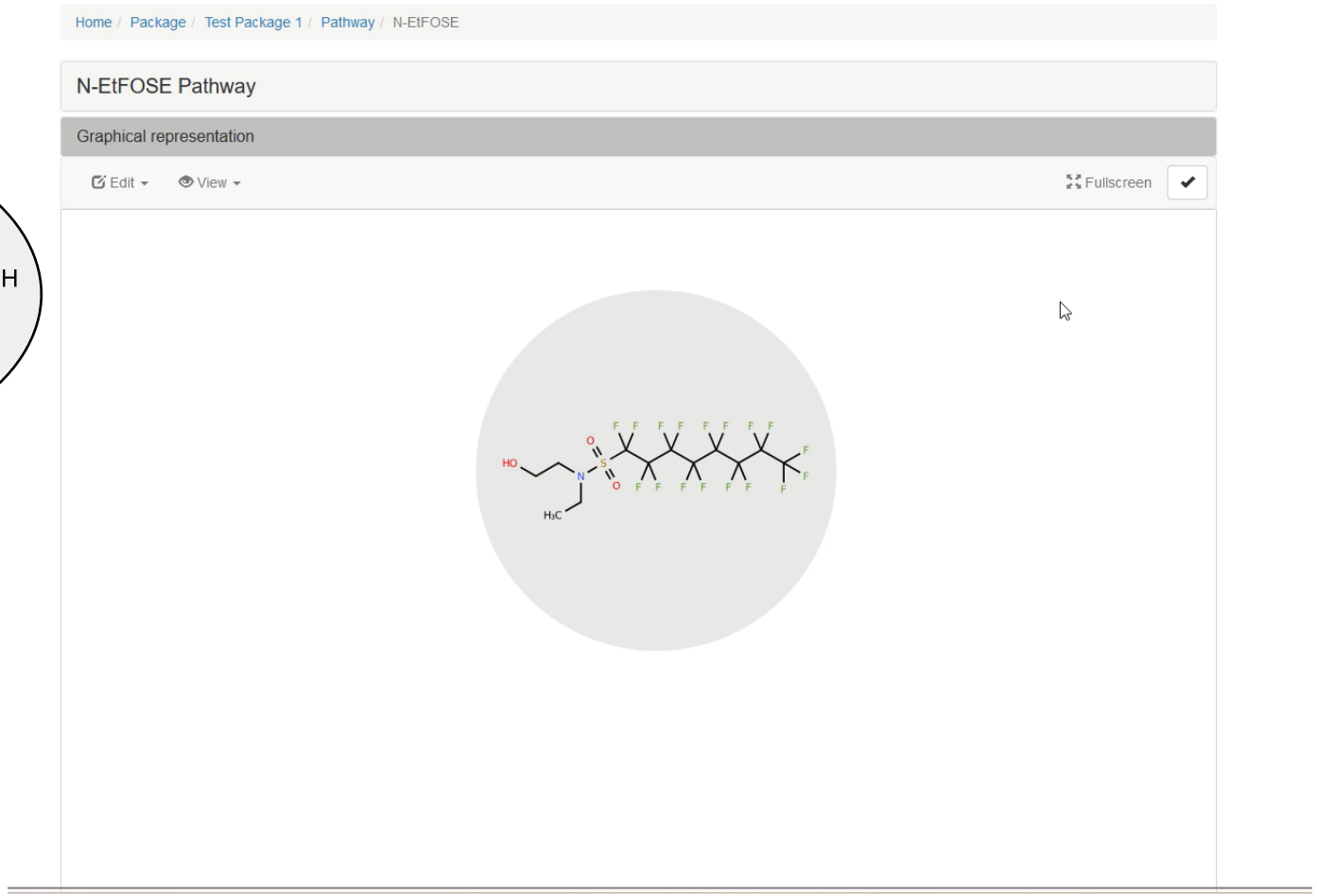


FIGURE 3. Proposed transformation pathway of *N*-EtFOSE in activated sludge.

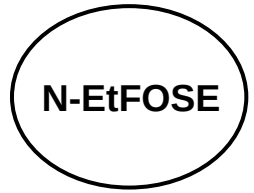


Rhoads, K. *et al*. Aerobic Biotransformation and Fate of N-Ethyl Perfluorooctane Sulfonamidoethanol (N-EtFOSE) in Activated Sludge. *Env. Sci. Tech.* **42**, 2873-2878 (2008).

Connect reactants (educts) with products

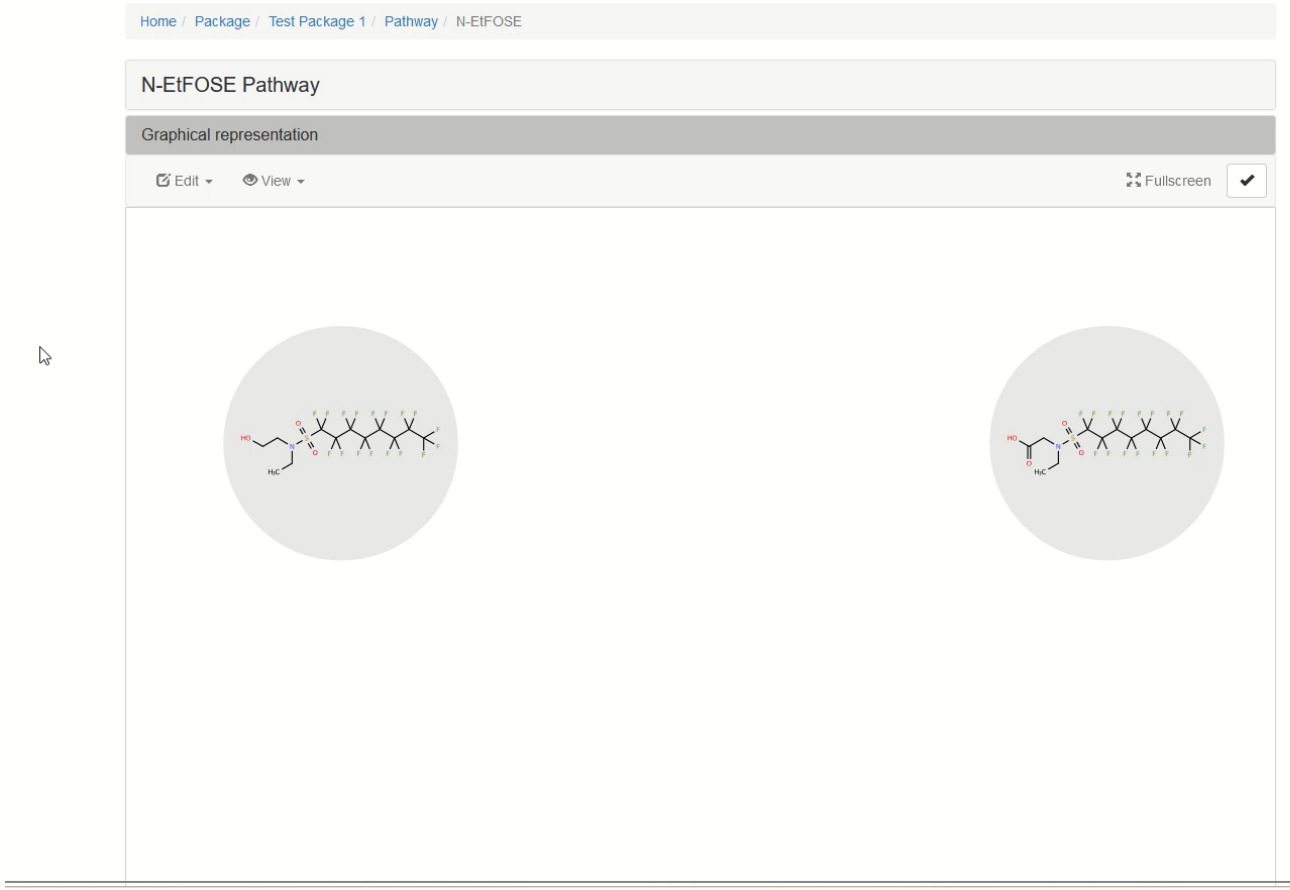
2

Parent compound



Transformation product A

Transformation product B



Add experimental information to the pathway using scenarios

2

Create a new empty scenario → Add experimental information

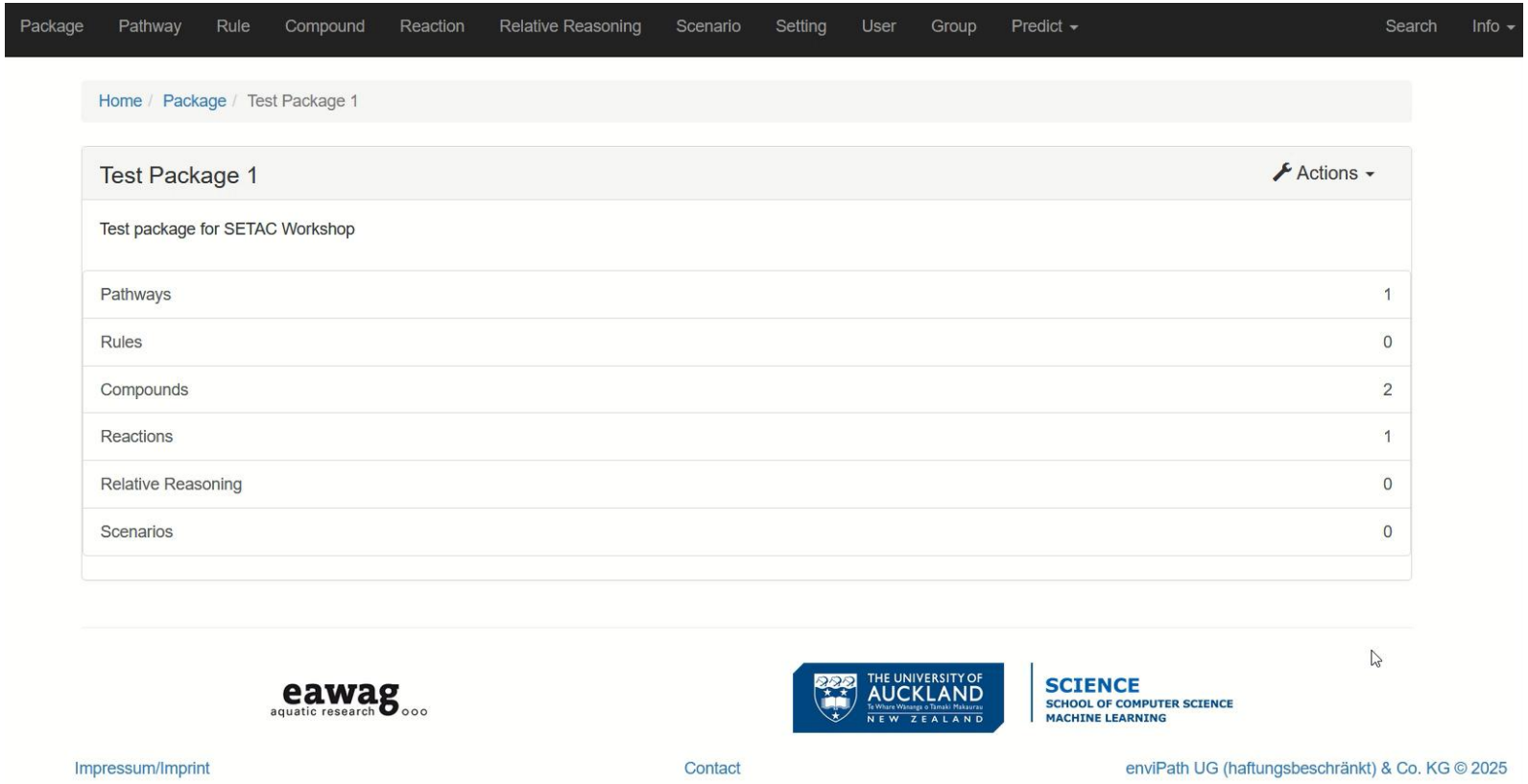
Text from paper
"Fresh **aerobic** activated sludge (**volatile suspended solids** 3.8 g/L) was obtained from the aeration basin at the Palo Alto WWTP in **Palo Alto, California**"

Rhoads, K. *et al*. Aerobic Biotransformation and Fate of N-Ethyl Perfluorooctane Sulfonamidoethanol (N-EtFOSE) in Activated Sludge. *Env. Sci. Tech.* **42**, 2873-2878 (2008).

Add experimental information to the pathway using scenarios

2

Scenario entries
Redox Condition - aerobic **Volatile suspended solids (VSS)** - 3.8 g/L **Location** - Palo Alto, CA



Add experimental information to the pathway using scenarios

2

Add more experimental information

Text from paper
"The observed first-order **rate constant** for the disappearance of N-EtFOSE calculated from the linear regression in Figure 2 (R^2= 0.967), is k_{obs} = 0.99 ± 0.08 d^{-1}, corresponding to a **half-life** of 0.71 ± 0.06 d (Table 2)."

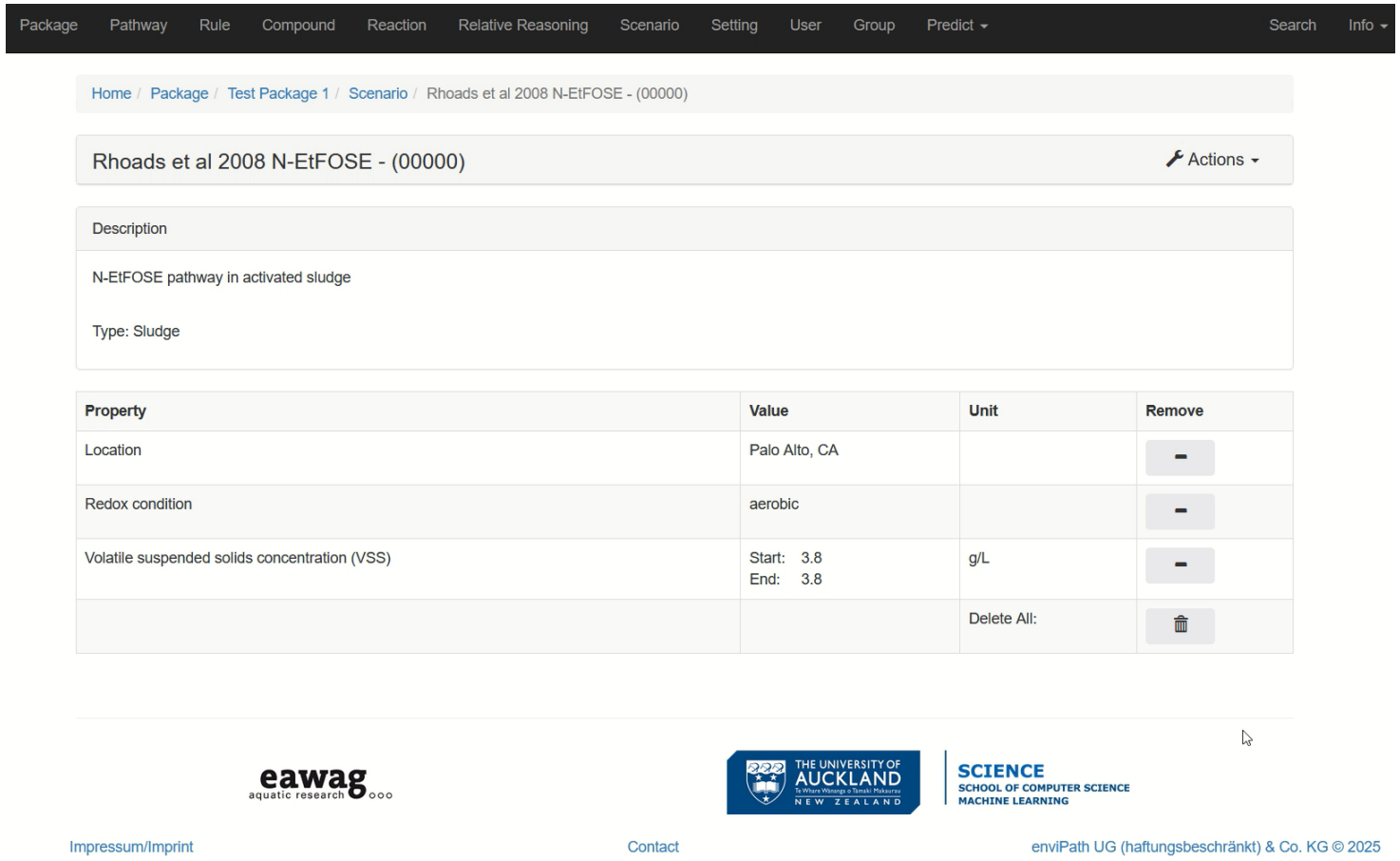
Rhoads, K. *et al*. Aerobic Biotransformation and Fate of N-Ethyl Perfluorooctane Sulfonamidoethanol (N-EtFOSE) in Activated Sludge. *Env. Sci. Tech.* **42**, 2873-2878 (2008).

Add experimental information to the pathway using scenarios

2

Scenario entries

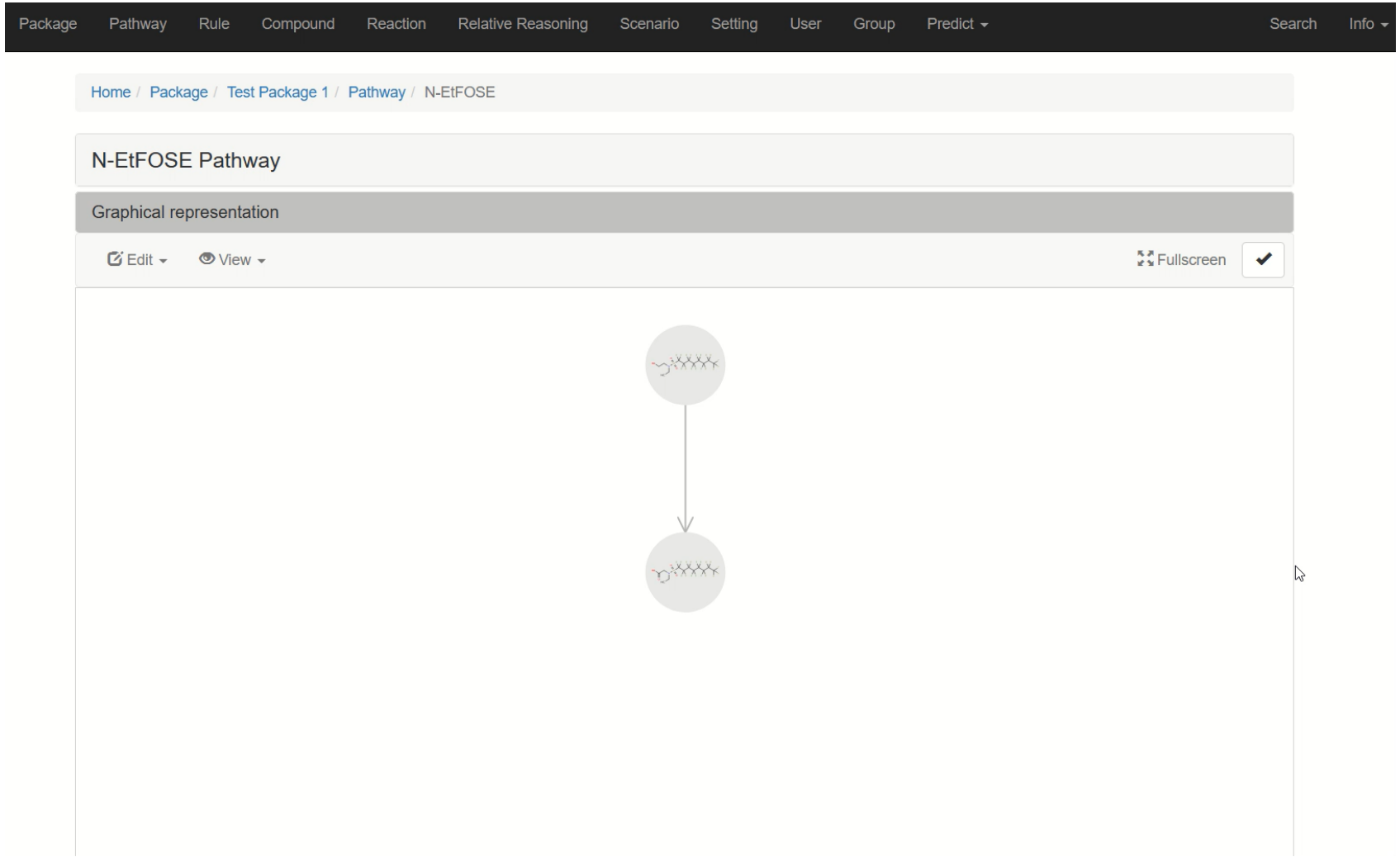
Rate constant
-Lower = 0.91 d^{-1}
-Upper = 1.07 d^{-1}
Half-life
-Lower = 0.65 d
-Upper = 0.77 d
-Fit = 0.967



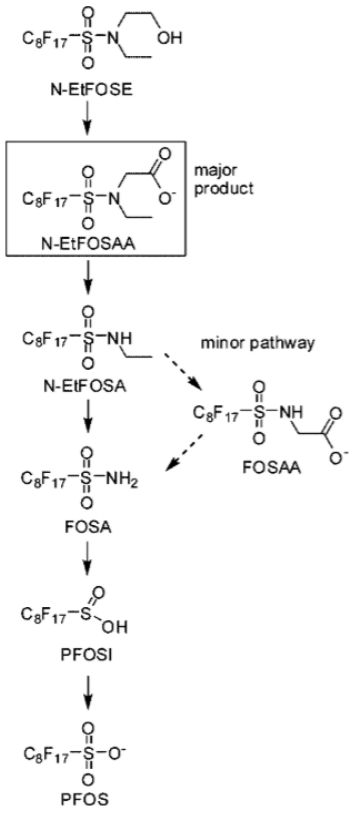
Add experimental information to the pathway using scenarios

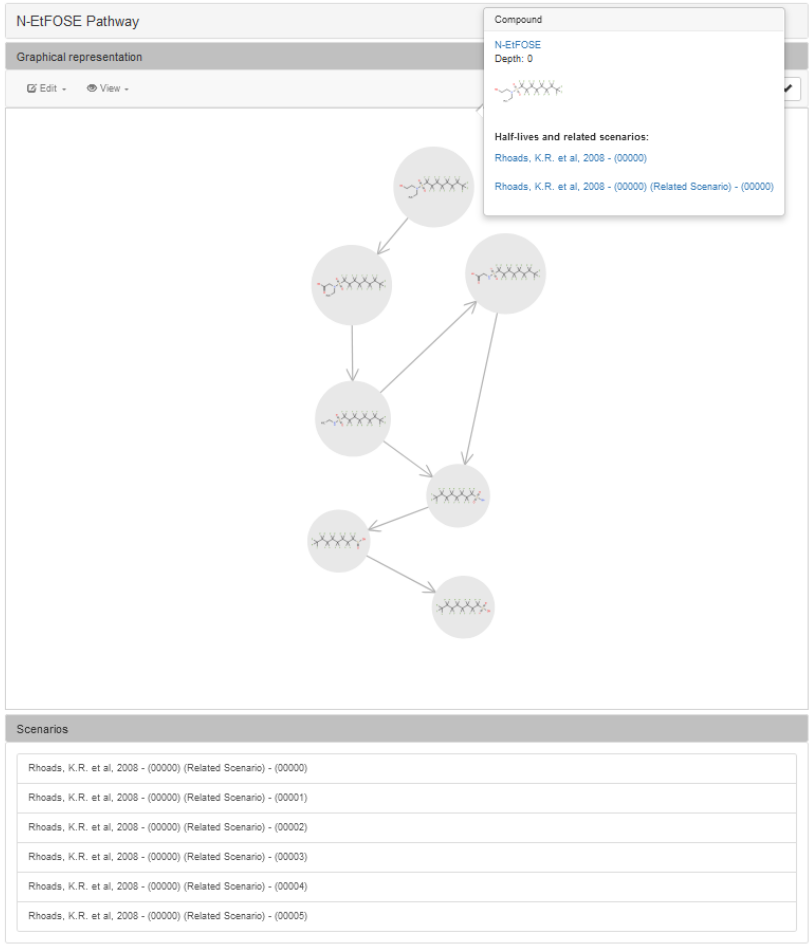
2

Attach the scenario to a compound in the pathway

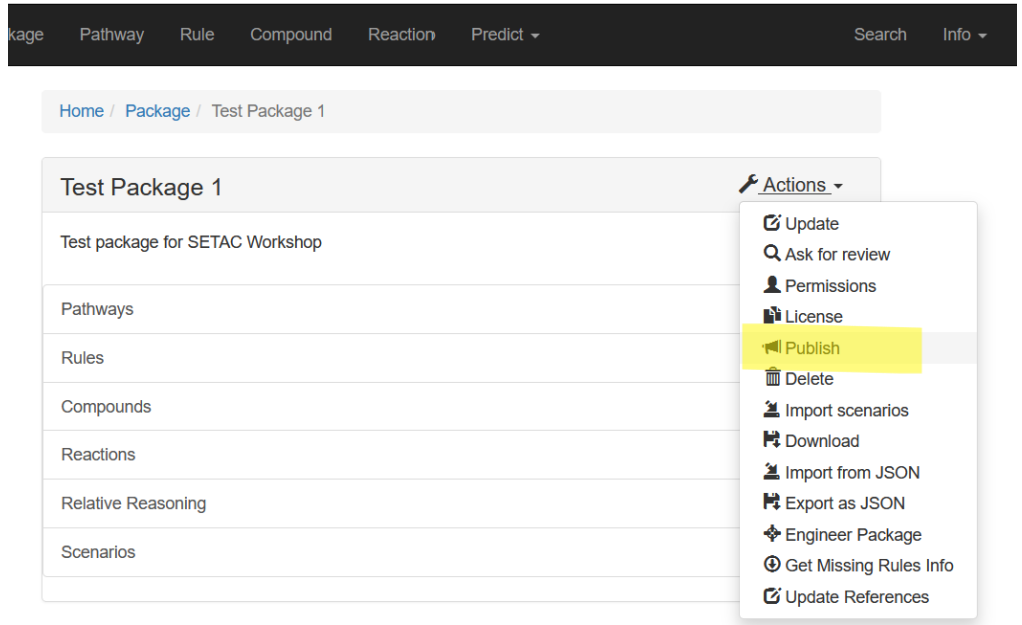


The Final Pathway





3 Make package public



Adding data for large datasets can get tedious…

1

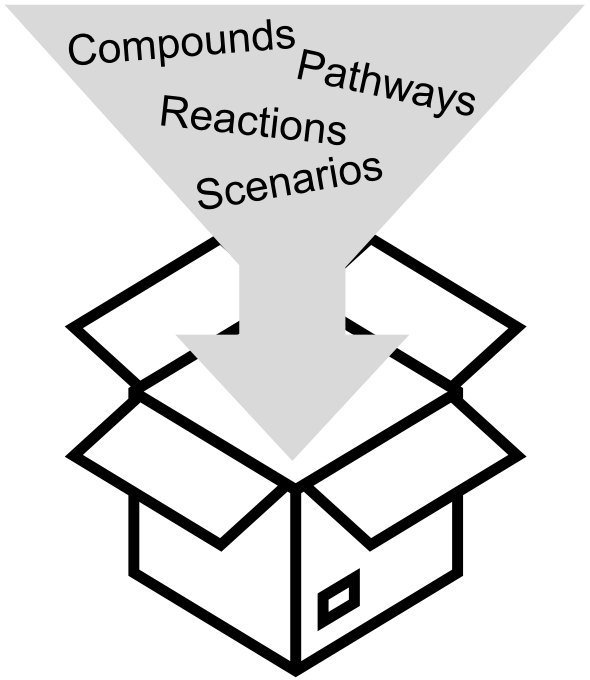
Create an empty package

2

Add your data to the empty package

3

Make package public



Where does your data come from?

"We built our random-forest model using the enviPath-PFAS package in addition to our own experimental data"

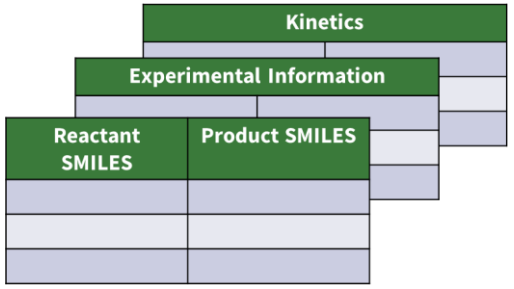
We require you to publish your data in a FAIR format

"Our dataset is publicly available on the enviPath platform"

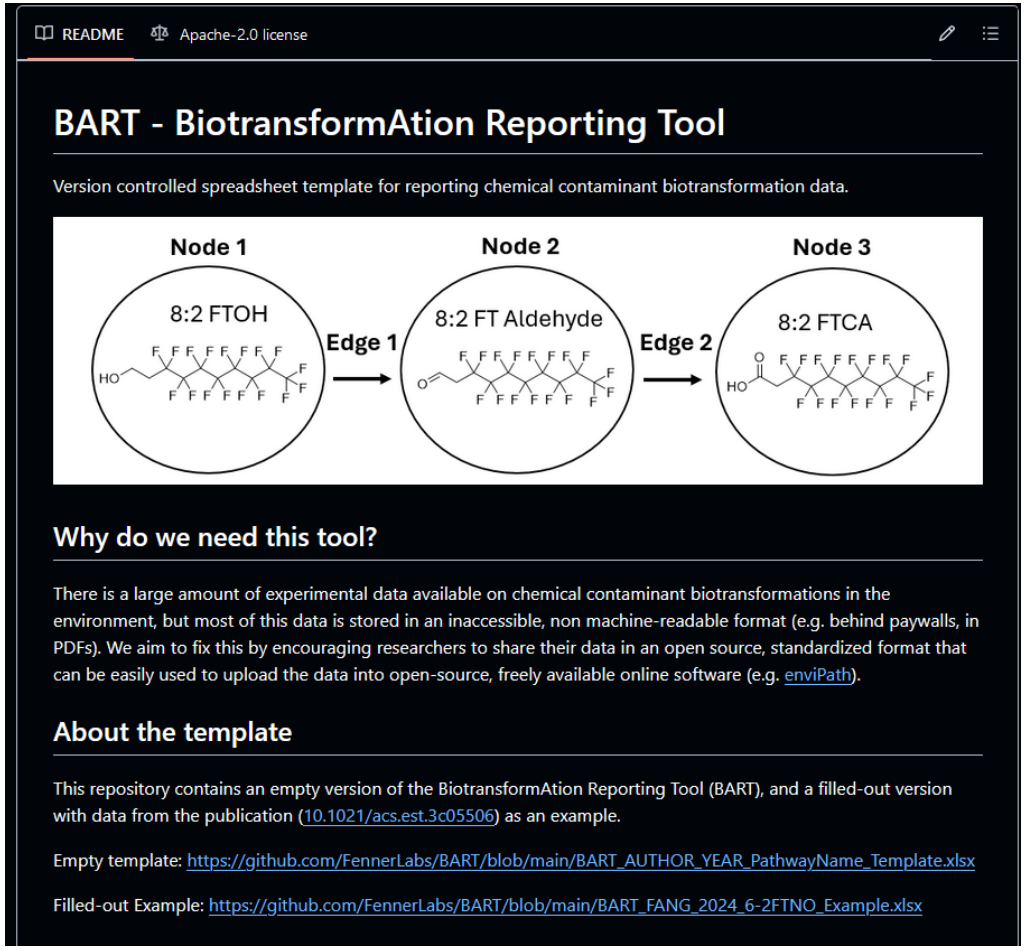
We developed a BiotransformAtion Reporting Tool (BART) to help upload pathways

Find it on GitHub

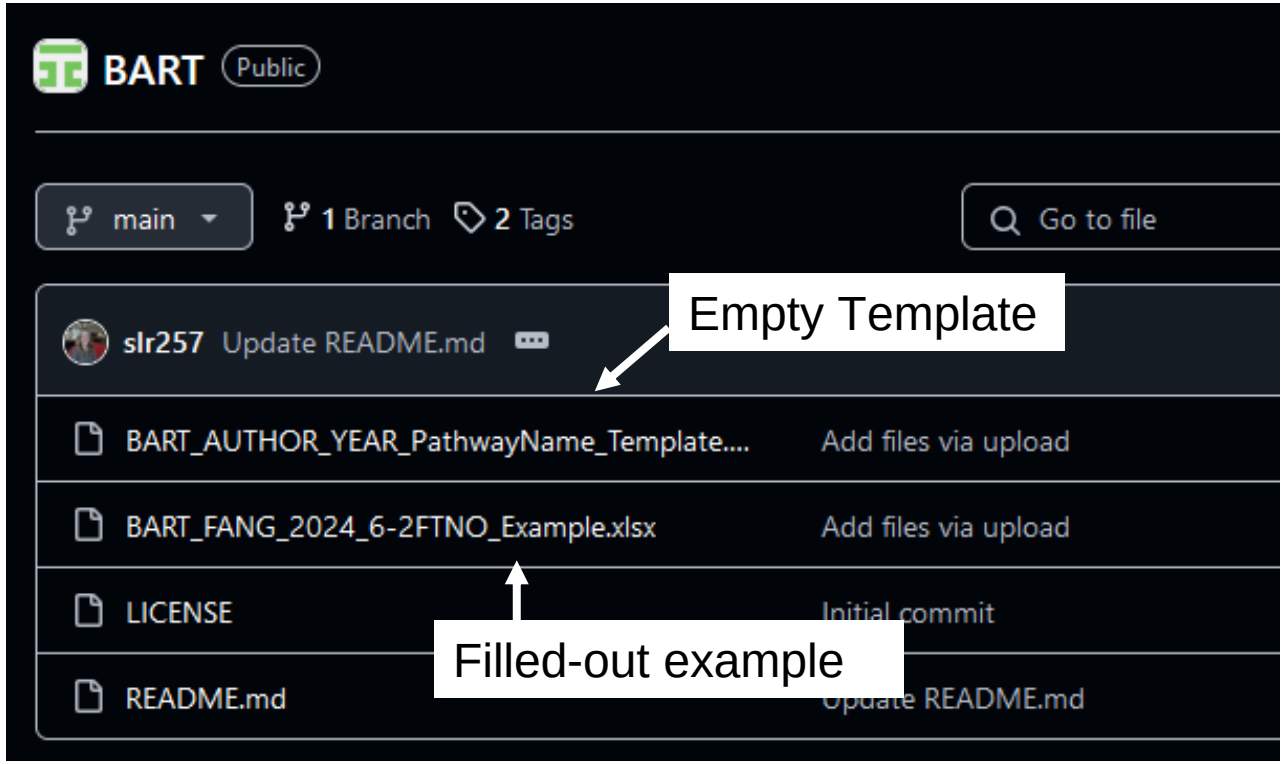
https://github.com/FennerLabs/BART



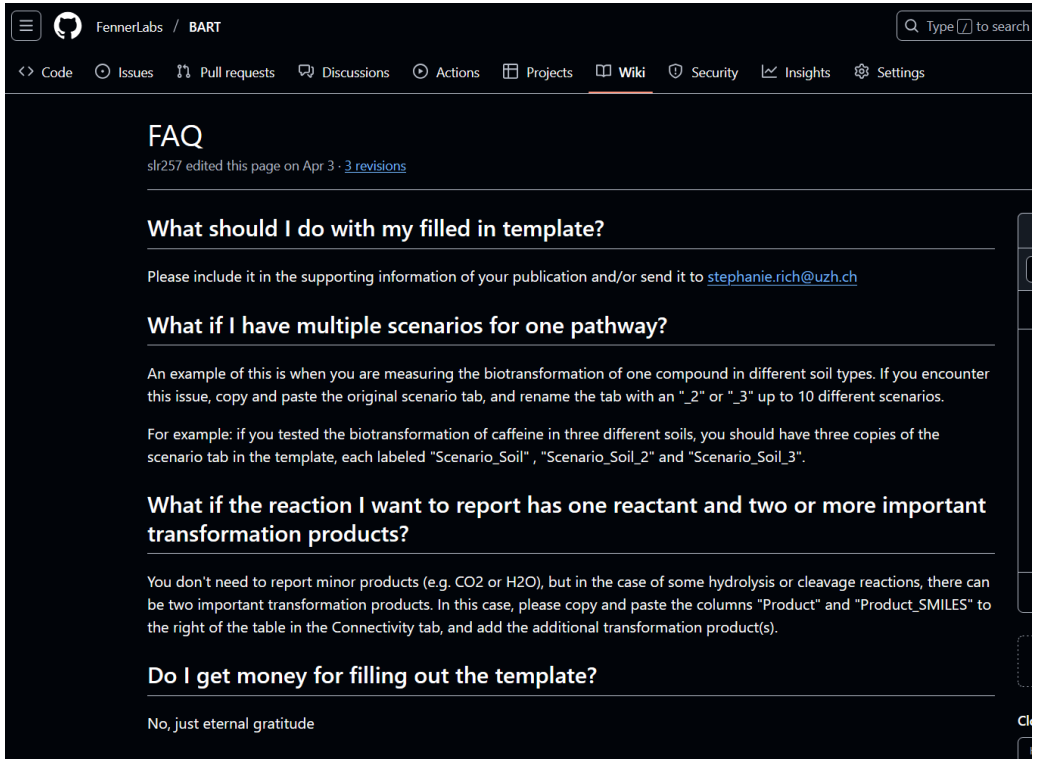
- Spreadsheet-based
- Compatible with enviPath Python
- Easy to edit and reuse



You can download and empty version and a filled-out example at the GitHub repository



There is a FAQ page in case you get stuck



BART also simplifies uploading large, complicated pathways

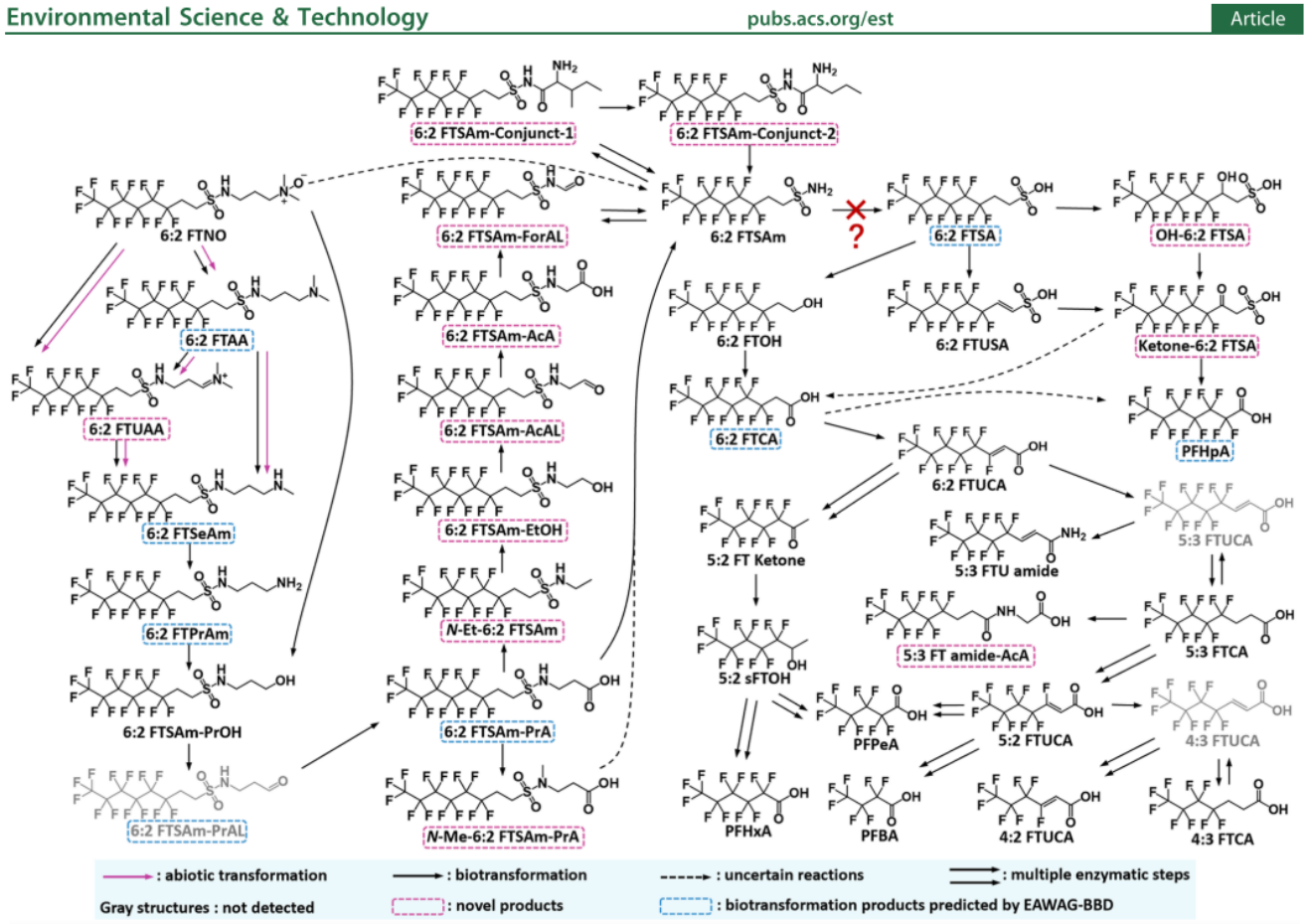


Figure 4. Proposed transformation pathways of 6:2 FTNO and 6:2 FTSA in aerobic sludge.

Fang, B. *et al.* Stability and Biotransformation of 6:2 Fluorotelomer Sulfonic Acid, Sulfonamide Amine Oxide, and Sulfonamide Alkylbetaine in Aerobic Sludge. *Env. Sci. Tech.* **58**, 2446-2457 (2024).

Filling out BART – Start with the Description Tab

Information	Entry
Paper Title	Stability and Biotransformation of 6:2 Fluorotelomer Sulfonic Acid, Sulfonamide Amine Oxide, and Sulfonamide Alkylbetaine in Aerobic Sludge
DOI	10.1021/acs.est.3c05506
Scenario Environment	Sludge
Your Name	Stephanie Rich
Email Address	stephanie.rich@uzh.ch
University/Company	University of Zürich

enviPath Pathway Upload Template

This workbook is designed to simplify the upload of biotransformation pathways into the enviPath database and pathway predition system (https://envipath.org/).

There are four main types of tabs (colored red and orange) in this workbook that should be filled out with an observed biotransformation pathway for one compound in one published study:

First, fill out the information in the **yellow highlighted table** in top left-hand corner. Next, fill out the tabs according to the description below:

Tab 1) **Compounds**: fill out this tab with compound types (parent or TP), names, and SMILES.

Tab 2) **Connectivity**: This tab defines observed biotransformation reactions from reactant to product using SMILES.

Tabs 3-6) **Scenarios**: These tab contain information about the environmental conditions at which the biotransformations were measured/observed. Pick the scenario type that best fits the environmental conditions in your paper, and designate this in the yellow highligted table in the top left-hand corner of this sheet.

Tab 7) **Kinetics_Confidence**: Biotransformation rate constants, half-lives, confidence levels, and proposed intermediates can be reported/designated here.

Additional tips for filling out this template:

* The template contains example data in each tab. Please replace this information with your new data.

* Cells colored in blue are drop-down lists.

* Cells colored in green can accept any input text or numerical values

* If something is confusing or does not fit your data, please write a comment in the "comment" column at the end of each table.

Please include a short description of the study used to generate the information in this excel workbook.

Data here are from the paper "Stability and Biotransformation of 6:2 Fluorotelomer Sulfonic Acid, Sulfonamide Amine Oxide, and Sulfonamide Alkylbetaine in Aerobic Sludge" (10.1021/acs.est.3c05506)

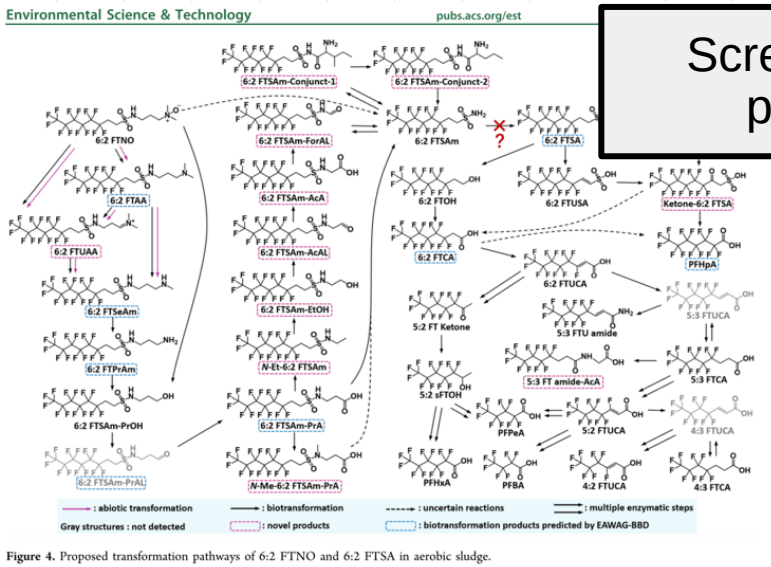


Figure 4. Proposed transformation pathways of 6:2 FTNO and 6:2 FTSA in aerobic sludge.

Description | Compounds | Connectivity | Scenario_Sludge | Scenario_Soil | Scenario_Water-Sediment | Scenario_General | Kinetics_Confidence

Name of paper, DOI, and template author information

Screenshot of pathway

Tabs represent different enviPath objects

Add SMILES for compounds in Compounds tab

Parent compound is clearly labeled

	A	B	C	D	E
1	**Type**	**Name**	**SMILES**		
2	Parent	6:2 FTNO	C[N+](C)(CCCNS(=O)(=O)CCC(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)[O-]		
3	TP	6:2 FTAA	FC(F)(C(C(C(C(C(CCS(=O)(=O)NCCCN(C)C)(F)F)(F)F)(F)F)(F)F)(F)F)F		
		6:2 FTUAA	FC(F)(C(C(C(C(C(C(CCS(=O)(=O)NCC/C=[N+](\C)/C)(F)F)(F)F)(F)F)(F)F)(F)F)F		
		6:2 FTSeAm	FC(F)(C(C(C(C(C(C(CCS(=O)(=O)NCCCNC)(F)F)(F)F)(F)F)(F)F)(F)F)F		
		6:2 FTPrAm	FC(F)(C(C(C(C(C(C(CCS(=O)(=O)NCCCN)(F)F)(F)F)(F)F)(F)F)(F)F)F		
		6:2 FTSAm-PrOH	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NCCCO)(=O)=O)F		
		6:2 FTSAm-PrAL	FC(F)(C(C(C(C(C(C(CCS(=O)(=O)NCCC=O)(F)F)(F)F)(F)F)(F)F)(F)F)F		
		6:2 FTSAm-PrA	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NCCC(O)=O)(=O)=O)F		
10	TP	N-Me-6:2 FTSAm-PrA	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(N(C)CCC(O)=O)(=O)=O)F		
11	TP	N-Et-6:2 FTSAm	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NCC)(=O)=O)F		
12	TP	6:2 FTSAm-EtOH	FC(C(F)(C(F)(C(F)(C(F)(C(F)(CCS(NCCO)(=O)=O)F)F)F)F)F)(F)F		
13	TP	6:2 FTSAm-AcAL	FC(C(F)(C(F)(C(F)(C(F)(C(F)(CCS(NCC=O)(=O)=O)F)F)F)F)F)(F)F		
14	TP	6:2 FTSAm-AcA	FC(C(F)(C(F)(C(F)(C(F)(C(F)(CCS(NCC(O)=O)(=O)=O)F)F)F)F)F)(F)F		
15	TP	6:2 FTSAm-ForAL	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NC=O)(=O)=O)F		
16	TP	6:2 FTSAm	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(N)(=O)=O)F		
17	TP	6:2 FTSAm-Conjunct-1	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NC(C(N)C(C)CC)=O)(=O)=O)F		
18	TP	6:2 FTSAm-Conjunct-2	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NC(C(N)CCC)=O)(=O)=O)F		
19					
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35					

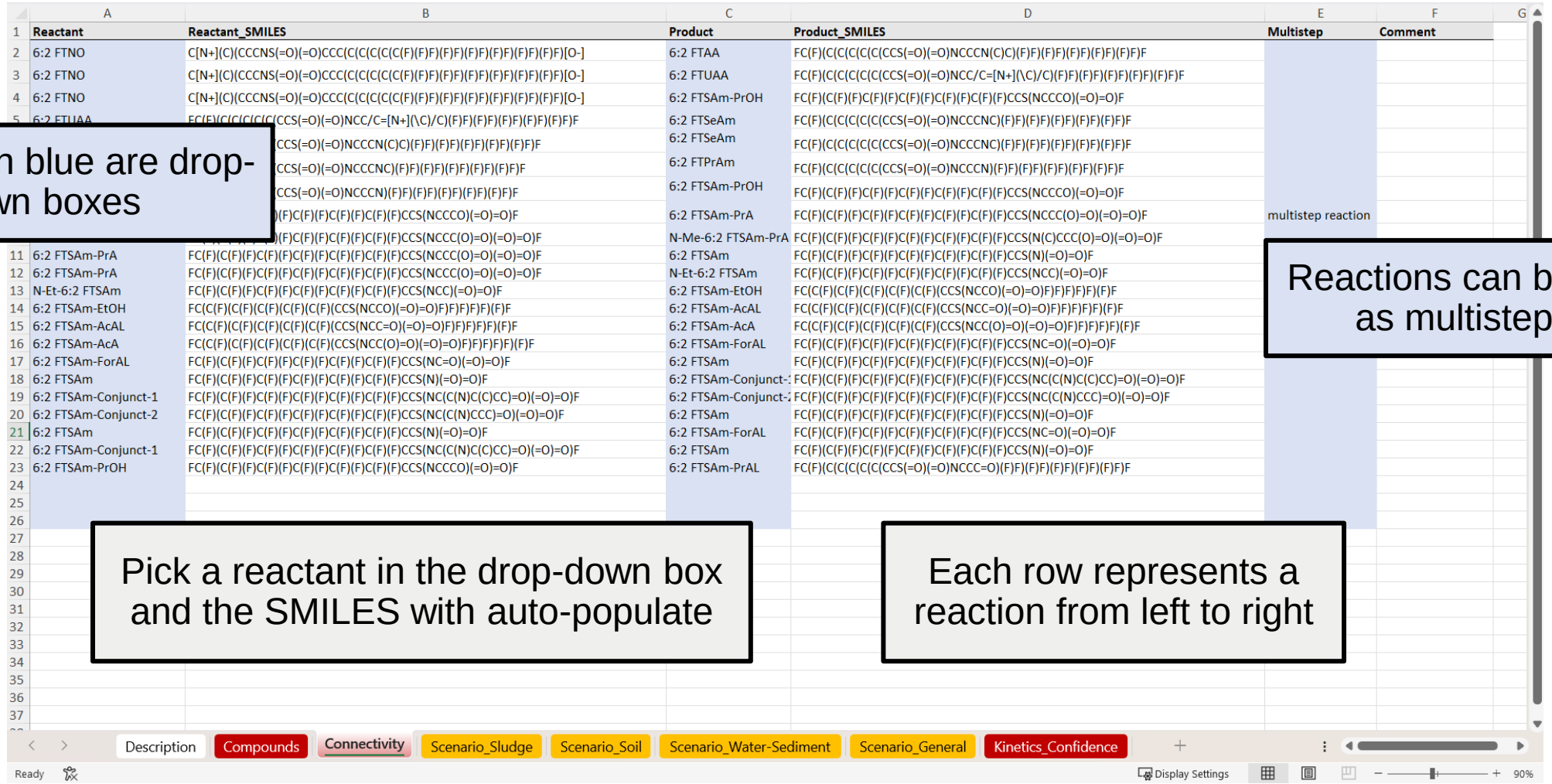
Description | Compounds | Connectivity | Scenario_Sludge | Scenario_Soil | Scenario_Water-Sediment | Scenario_General | Kinetics_Confidence

Ready | Display Settings

SMILES for all compounds in a pathway should be provided in one column with each corresponding compound name

Connect Reactants and Products in the Connectivity Tab

Columns in blue are drop-down boxes



	A	B	C	D	E	F	G
1	Reactant	Reactant_SMILES	Product	Product_SMILES	Multistep	Comment	
2	6:2 FTNO	C[N+](C)(CCCNS(=O)(=O)CCC(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)[O-]	6:2 FTAA	FC(F)(C(C(C(C(C(CCS(=O)(=O)NCCCN(C)C)(F)F)(F)F)(F)F)(F)F)(F)F)F			
3	6:2 FTNO	C[N+](C)(CCCNS(=O)(=O)CCC(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)[O-]	6:2 FTUAA	FC(F)(C(C(C(C(C(CCS(=O)(=O)NCC/C=[N+]\(\C)/C)(F)F)(F)F)(F)F)(F)F)(F)F)F			
4	6:2 FTNO	C[N+](C)(CCCNS(=O)(=O)CCC(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)[O-]	6:2 FTSAm-PrOH	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NCCCO)(=O)=O)F			
5	6:2 FTUAA	FC(F)(C(C(C(C(C(CCS(=O)(=O)NCC/C=[N+](\C)/C)(F)F)(F)F)(F)F)(F)F)(F)F)F	6:2 FTSeAm	FC(F)(C(C(C(C(C(CCS(=O)(=O)NCCCNC)(F)F)(F)F)(F)F)(F)F)(F)F)F			
		(CCS(=O)(=O)NCCCN(C)C)(F)F)(F)F)(F)F)(F)F)(F)F)F	6:2 FTSeAm	FC(F)(C(C(C(C(C(CCS(=O)(=O)NCCCNC)(F)F)(F)F)(F)F)(F)F)(F)F)F			
		(CCS(=O)(=O)NCCCNC)(F)F)(F)F)(F)F)(F)F)(F)F)F	6:2 FTPrAm	FC(F)(C(C(C(C(C(CCS(=O)(=O)NCCCN)(F)F)(F)F)(F)F)(F)F)(F)F)F			
		(CCS(=O)(=O)NCCCN)(F)F)(F)F)(F)F)(F)F)(F)F)F	6:2 FTSAm-PrOH	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NCCCO)(=O)=O)F			
		)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NCCCO)(=O)=O)F	6:2 FTSAm-PrA	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NCCC(O)=O)(=O)=O)F	multistep reaction		
		)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NCCC(O)=O)(=O)=O)F	N-Me-6:2 FTSAm-PrA	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(N(C)CCC(O)=O)(=O)=O)F			
11	6:2 FTSAm-PrA	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NCCC(O)=O)(=O)=O)F	6:2 FTSAm	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(N)(=O)=O)F			
12	6:2 FTSAm-PrA	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NCCC(O)=O)(=O)=O)F	N-Et-6:2 FTSAm	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NCC)(=O)=O)F			
13	N-Et-6:2 FTSAm	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NCC)(=O)=O)F	6:2 FTSAm-EtOH	FC(C(F)(C(F)(C(F)(C(F)(C(F)(C(F)(CCS(NCCO)(=O)=O)F)F)F)F)F)F)(F)F			
14	6:2 FTSAm-EtOH	FC(C(F)(C(F)(C(F)(C(F)(C(F)(C(F)(CCS(NCCO)(=O)=O)F)F)F)F)F)F)(F)F	6:2 FTSAm-AcAL	FC(C(F)(C(F)(C(F)(C(F)(C(F)(C(F)(CCS(NCC=O)(=O)=O)F)F)F)F)F)F)(F)F			
15	6:2 FTSAm-AcAL	FC(C(F)(C(F)(C(F)(C(F)(C(F)(C(F)(CCS(NCC=O)(=O)=O)F)F)F)F)F)F)(F)F	6:2 FTSAm-AcA	FC(C(F)(C(F)(C(F)(C(F)(C(F)(C(F)(CCS(NCC(O)=O)(=O)=O)F)F)F)F)F)F)(F)F			
16	6:2 FTSAm-AcA	FC(C(F)(C(F)(C(F)(C(F)(C(F)(C(F)(CCS(NCC(O)=O)(=O)=O)F)F)F)F)F)F)(F)F	6:2 FTSAm-ForAL	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NC=O)(=O)=O)F			
17	6:2 FTSAm-ForAL	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NC=O)(=O)=O)F	6:2 FTSAm	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(N)(=O)=O)F			
18	6:2 FTSAm	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(N)(=O)=O)F	6:2 FTSAm-Conjunct-1	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NC(C(N)C(C)CC)=O)(=O)=O)F			
19	6:2 FTSAm-Conjunct-1	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NC(C(N)C(C)CC)=O)(=O)=O)F	6:2 FTSAm-Conjunct-2	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NC(C(N)CCC)=O)(=O)=O)F			
20	6:2 FTSAm-Conjunct-2	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NC(C(N)CCC)=O)(=O)=O)F	6:2 FTSAm	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(N)(=O)=O)F			
21	6:2 FTSAm	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(N)(=O)=O)F	6:2 FTSAm-ForAL	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NC=O)(=O)=O)F			
22	6:2 FTSAm-Conjunct-1	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NC(C(N)C(C)CC)=O)(=O)=O)F	6:2 FTSAm	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(N)(=O)=O)F			
23	6:2 FTSAm-PrOH	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NCCCO)(=O)=O)F	6:2 FTSAm-PrAL	FC(F)(C(C(C(C(C(CCS(=O)(=O)NCCC=O)(F)F)(F)F)(F)F)(F)F)(F)F)F			
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Description | Compounds | Connectivity | Scenario_Sludge | Scenario_Soil | Scenario_Water-Sediment | Scenario_General | Kinetics_Confidence

Ready | Display Settings | 90%

Reactions can be flagged as multistep here

Pick a reactant in the drop-down box and the SMILES with auto-populate

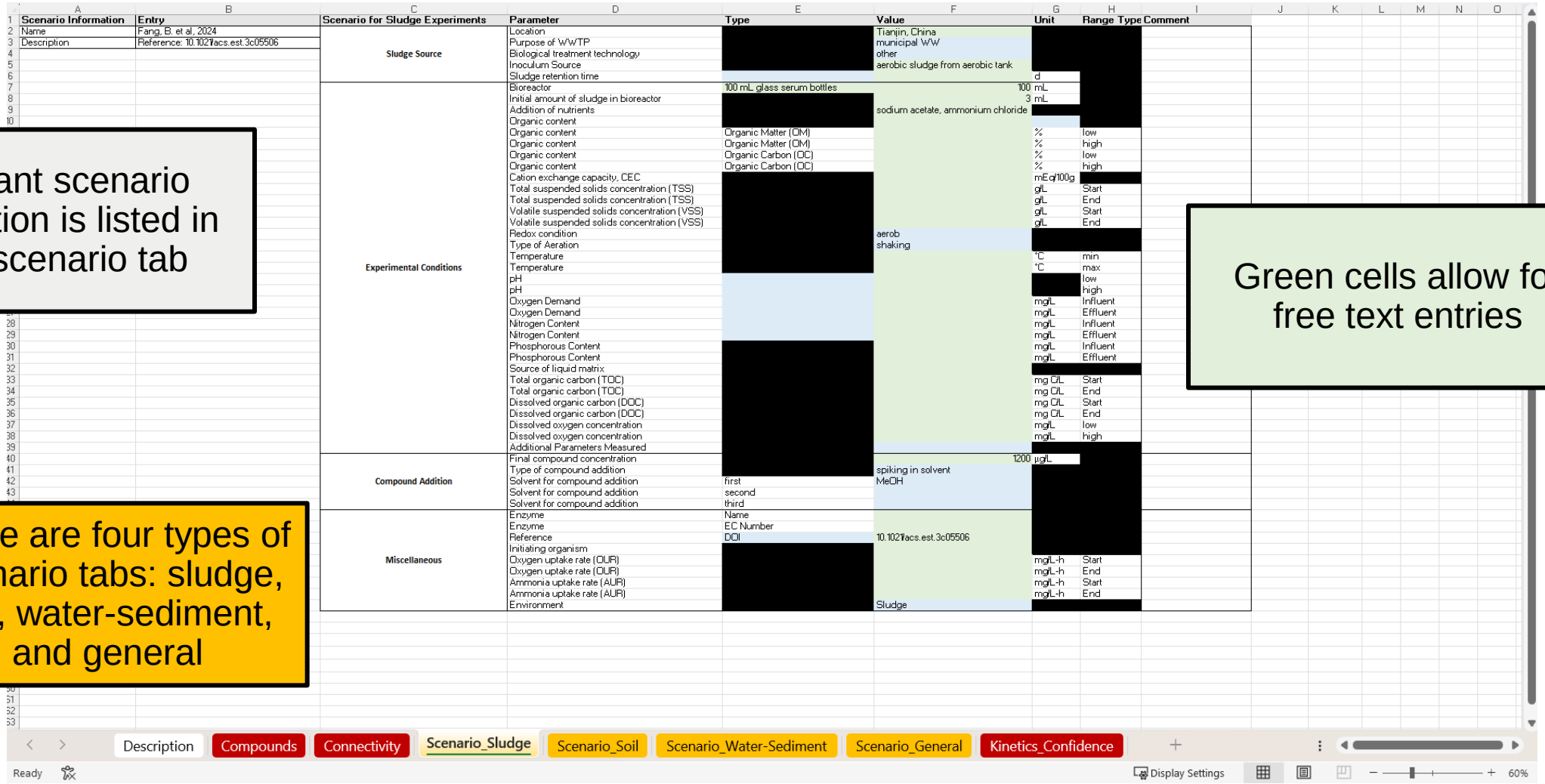
Each row represents a reaction from left to right

Fill-out Scenario information in a tabular format

Relevant scenario information is listed in each scenario tab

There are four types of scenario tabs: sludge, soil, water-sediment, and general

Green cells allow for free text entries



Scenario Information	Entry
Name	Fang, B. et al, 2024
Description	Reference: 10.1021/acs.est.3c05506

Scenario for Sludge Experiments	Parameter	Type	Value	Unit	Range Type	Comment
Sludge Source	Location		Tianjin, China			
	Purpose of WWTP		municipal WW			
	Biological treatment technology		other			
	Inoculum Source		aerobic sludge from aerobic tank			
	Sludge retention time			d		
Experimental Conditions	Bioreactor	100 mL glass serum bottles				
	Initial amount of sludge in bioreactor		100	mL		
	Addition of nutrients		3	mL		
	Organic content		sodium acetate, ammonium chloride			
	Organic content	Organic Matter (OM)		%	low	
	Organic content	Organic Matter (OM)		%	high	
	Organic content	Organic Carbon (OC)		%	low	
	Organic content	Organic Carbon (OC)		%	high	
	Cation exchange capacity, CEC			mEq/100g		
	Total suspended solids concentration (TSS)			g/L	Start	
	Total suspended solids concentration (TSS)			g/L	End	
	Volatile suspended solids concentration (VSS)			g/L	Start	
	Volatile suspended solids concentration (VSS)			g/L	End	
	Redox condition		aerob			
	Type of Aeration		shaking			
	Temperature			°C	min	
	Temperature			°C	max	
	pH				low	
	pH				high	
	Oxygen Demand			mg/L	Influent	
	Oxygen Demand			mg/L	Effluent	
	Nitrogen Content			mg/L	Influent	
	Nitrogen Content			mg/L	Effluent	
	Phosphorous Content			mg/L	Influent	
	Phosphorous Content			mg/L	Effluent	
	Source of liquid matrix					
	Total organic carbon (TOC)			mg C/L	Start	
	Total organic carbon (TOC)			mg C/L	End	
	Dissolved organic carbon (DOC)			mg C/L	Start	
	Dissolved organic carbon (DOC)			mg C/L	End	
	Dissolved oxygen concentration			mg/L	low	
	Dissolved oxygen concentration			mg/L	high	
	Additional Parameters Measured					
Compound Addition	Final compound concentration		1200	µg/L		
	Type of compound addition		spiking in solvent			
	Solvent for compound addition	first	MeOH			
	Solvent for compound addition	second				
	Solvent for compound addition	third				
Miscellaneous	Enzyme	Name				
	Enzyme	EC Number				
	Reference	DOI	10.1021/acs.est.3c05506			
	Initiating organism					
	Oxygen uptake rate (OUR)			mg/L-h	Start	
	Oxygen uptake rate (OUR)			mg/L-h	End	
	Ammonia uptake rate (AUR)			mg/L-h	Start	
	Ammonia uptake rate (AUR)			mg/L-h	End	
	Environment		Sludge			

Description | Compounds | Connectivity | Scenario_Sludge | Scenario_Soil | Scenario_Water-Sediment | Scenario_General | Kinetics_Confidence

Ready | Display Settings | 60%

Add kinetics, confidence levels, and proposed intermediates last

Scenario	Compound	SMILES	Model	Parameter	Value	Value Unit	Corrected	R2	Confidence Level_PFAS	Confidence Level_Schy	Proposed Intermediate?	Comment
Fang, B. et al, 2024	6:2 FTNO	C[N+](C)(CCCNS(=O)(=O)CCC(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	SFO	Half-life	1.2	d		0.9976	1a	1		
Fang, B. et al, 2024	6:2 FTAA	FC(F)(C(C(C(C(C(CCS(=O)(=O)NCCCN(C)C)(F)F)(F)F)(F)F)(F)F)(F)F)F	SFO	Half-life	11.5	d		0.904	2a	2		
Fang, B. et al, 2024	6:2 FTUAA	FC(F)(C(C(C(C(C(CCS(=O)(=O)NCC/C=[N+](\C)/C)(F)F)(F)F)(F)F)(F)F)(F)F)F							2b	2		
Fang, B. et al, 2024	6:2 FTSeAm	FC(F)(C(C(C(C(C(CCS(=O)(=O)NCCCNC)(F)F)(F)F)(F)F)(F)F)(F)F)F							2a	2		
Fang, B. et al, 2024	6:2 FTPrAm	FC(F)(C(C(C(C(C(CCS(=O)(=O)NCCCN)(F)F)(F)F)(F)F)(F)F)(F)F)F							2c	2		
Fang, B. et al, 2024	6:2 FTSAm-PrOH	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NCCCO)(=O)=O)F							2a	2		
Fang, B. et al, 2024	6:2 FTSAm-PrA	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NCCC(O)=O)(=O)=O)F							2a	2		
Fang, B. et al, 2024	N-Me-6:2 FTSAm-PrA	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(N(C)CCC(O)=O)(=O)=O)F							3a	3		
Fang, B. et al, 2024	N-Et-6:2 FTSAm	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NCC)(=O)=O)F							2b	2		
Fang, B. et al, 2024	6:2 FTSAm-EtOH	FC(C(F)(C(F)(C(F)(C(F)(C(F)(CCS(NCCO)(=O)=O)F)F)F)F)F)(F)F							2b	2		
Fang, B. et al, 2024	6:2 FTSAm-AcAL	FC(C(F)(C(F)(C(F)(C(F)(C(F)(CCS(NCC=O)(=O)=O)F)F)F)F)F)(F)F							2b	2		
Fang, B. et al, 2024	6:2 FTSAm-AcA	FC(C(F)(C(F)(C(F)(C(F)(C(F)(CCS(NCC(O)=O)(=O)=O)F)F)F)F)F)(F)F							2b	2		
Fang, B. et al, 2024	6:2 FTSAm-ForAL	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NC=O)(=O)=O)F							2b	2		
Fang, B. et al, 2024	6:2 FTSAm	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(N)(=O)=O)F							2a	2		
Fang, B. et al, 2024	6:2 FTSAm-Conjunct-1	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NC(C(N)C(C)CC)=O)(=O)=O)F							3a	3		
Fang, B. et al, 2024	6:2 FTSAm-Conjunct-2	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS(NC(C(N)CCC)=O)(=O)=O)F							3a	3		
Fang, B. et al, 2024	6:2 FTSAm-PrAL	FC(F)(C(C(C(C(C(CCS(=O)(=O)NCCC=O)(F)F)(F)F)(F)F)(F)F)(F)F)F									proposed	

The last tab is for reporting half-lives, rate constants, identification confidence levels, and proposed intermediates

Description | Compounds | Connectivity | Scenario_Sludge | Scenario_Soil | Scenario_Water-Sediment | Scenario_General | Kinetics_Confidence

Ready

Display Settings

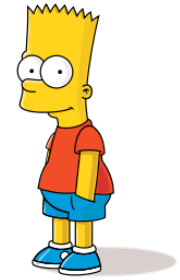
80%

What should you do with the finished BART?

1. Include BART in the Supporting Information of your manuscript at submission

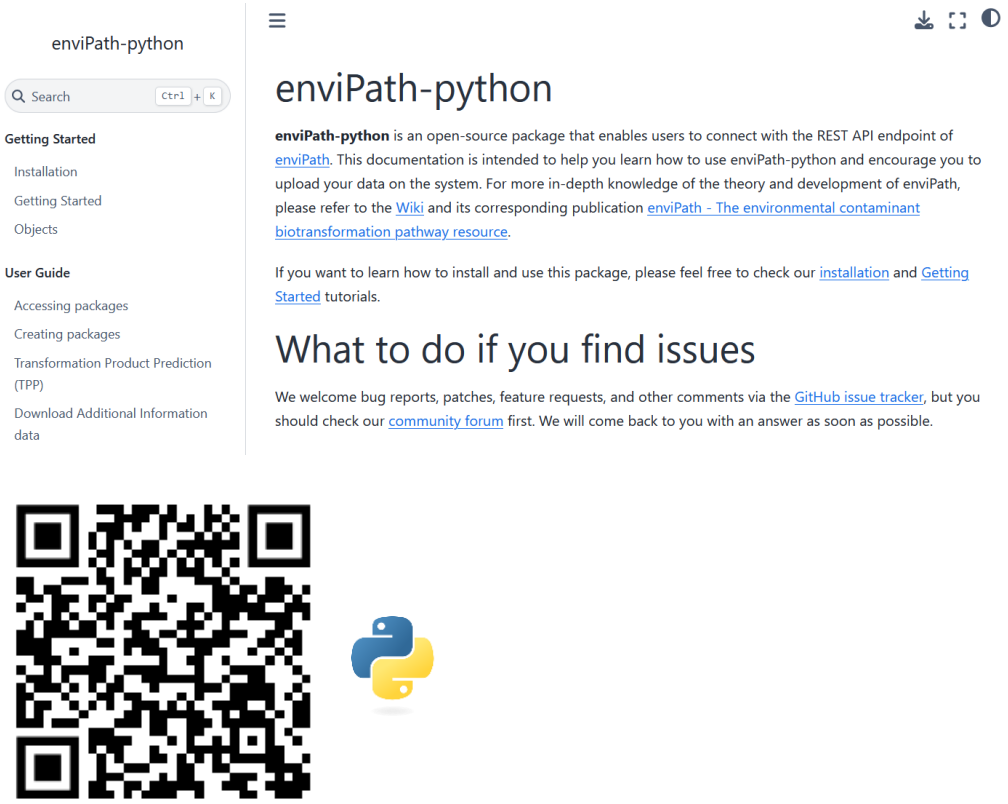
2. Send your BART files to the enviPath team (stephanie.rich@uzh.ch) and we can generate the package for you in 1-2 days

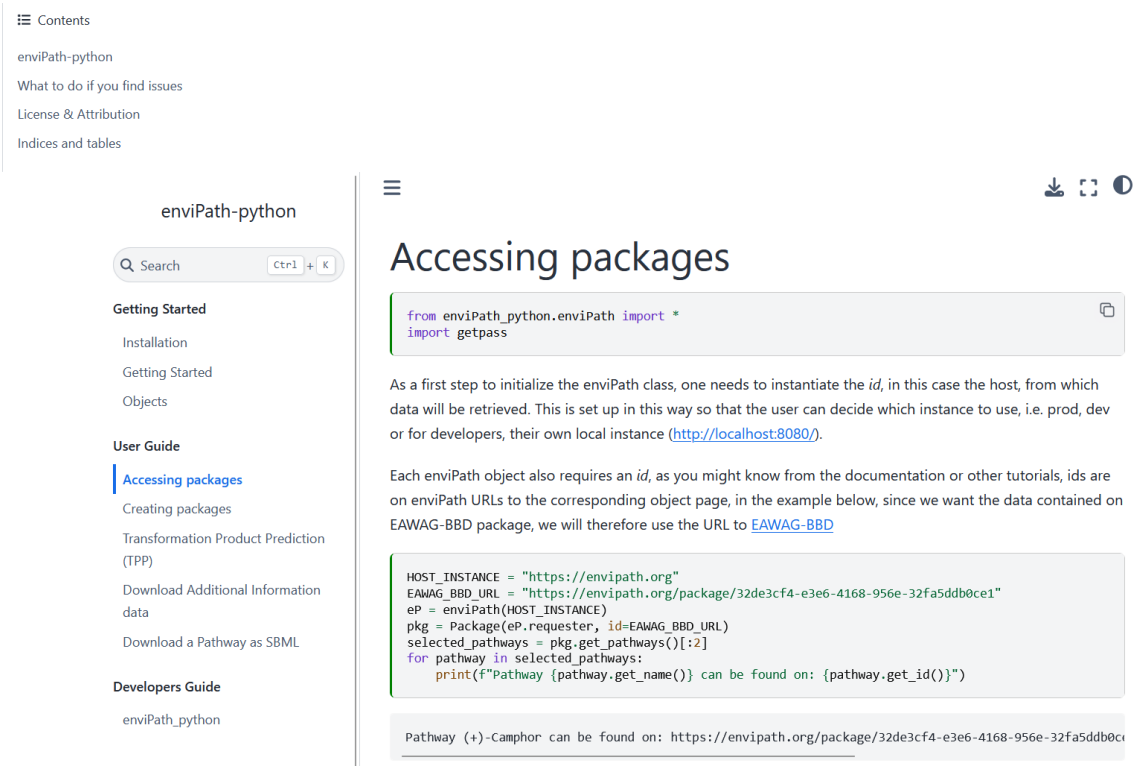
3. Upload your pathways using our command-line executable (this will be available at the GitHub repo soon)



Extracting data from enviPath currently requires knowledge of python, and we are working to make this more user-friendly

Please visit the tutorial website to try out enviPath Python





Acknowledgements

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eawag aquatic research

Questions?

Hands-On Example

Either follow along with our example, or try it on a pathway of your choice

Steps:

1. Find a paper with a biotransformation pathway
2. Go to BART and download and empty template