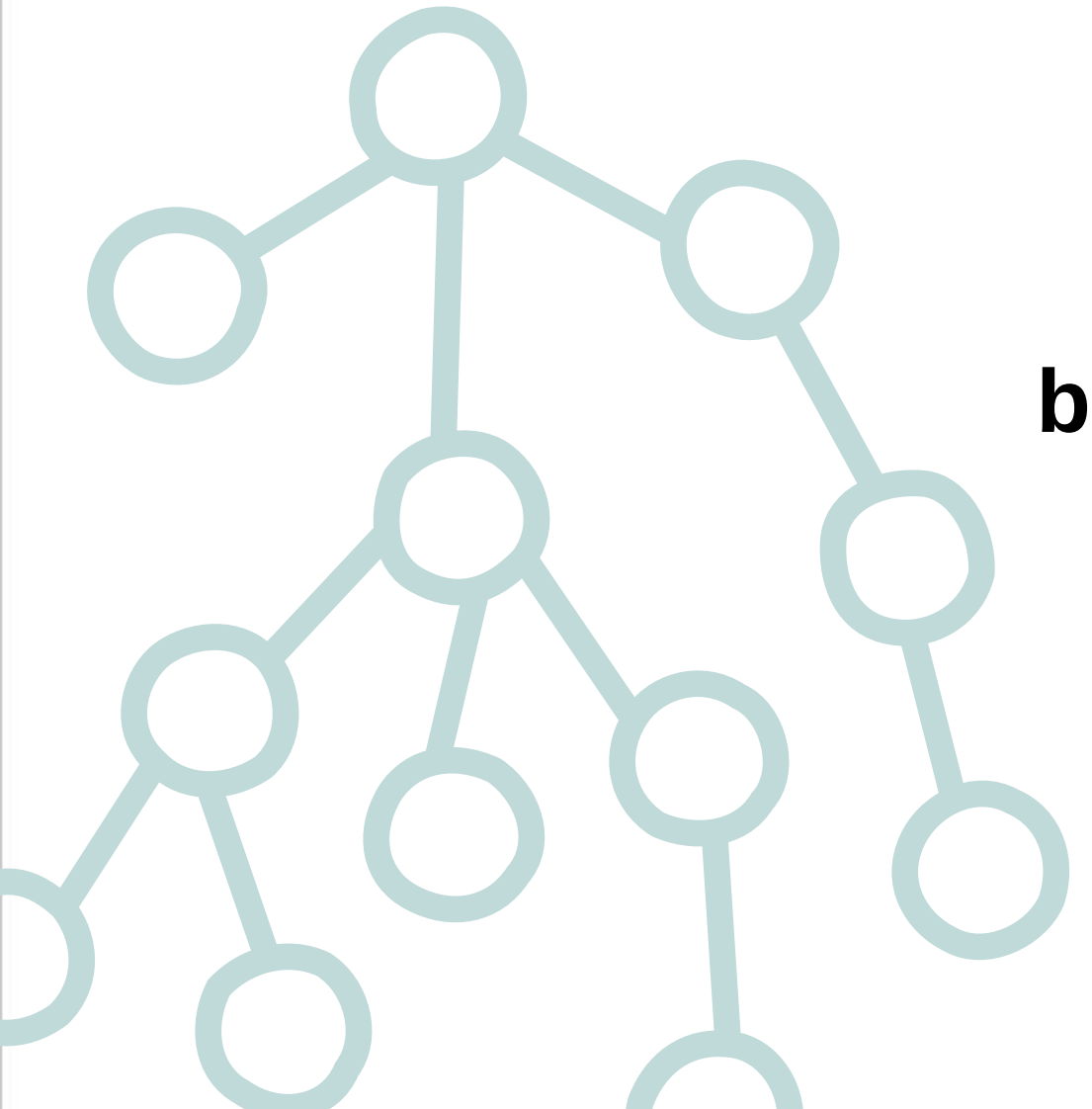
Universität Zürich[UZH]

Eawag
Swiss Federal Institute of Aquatic Science and Technology

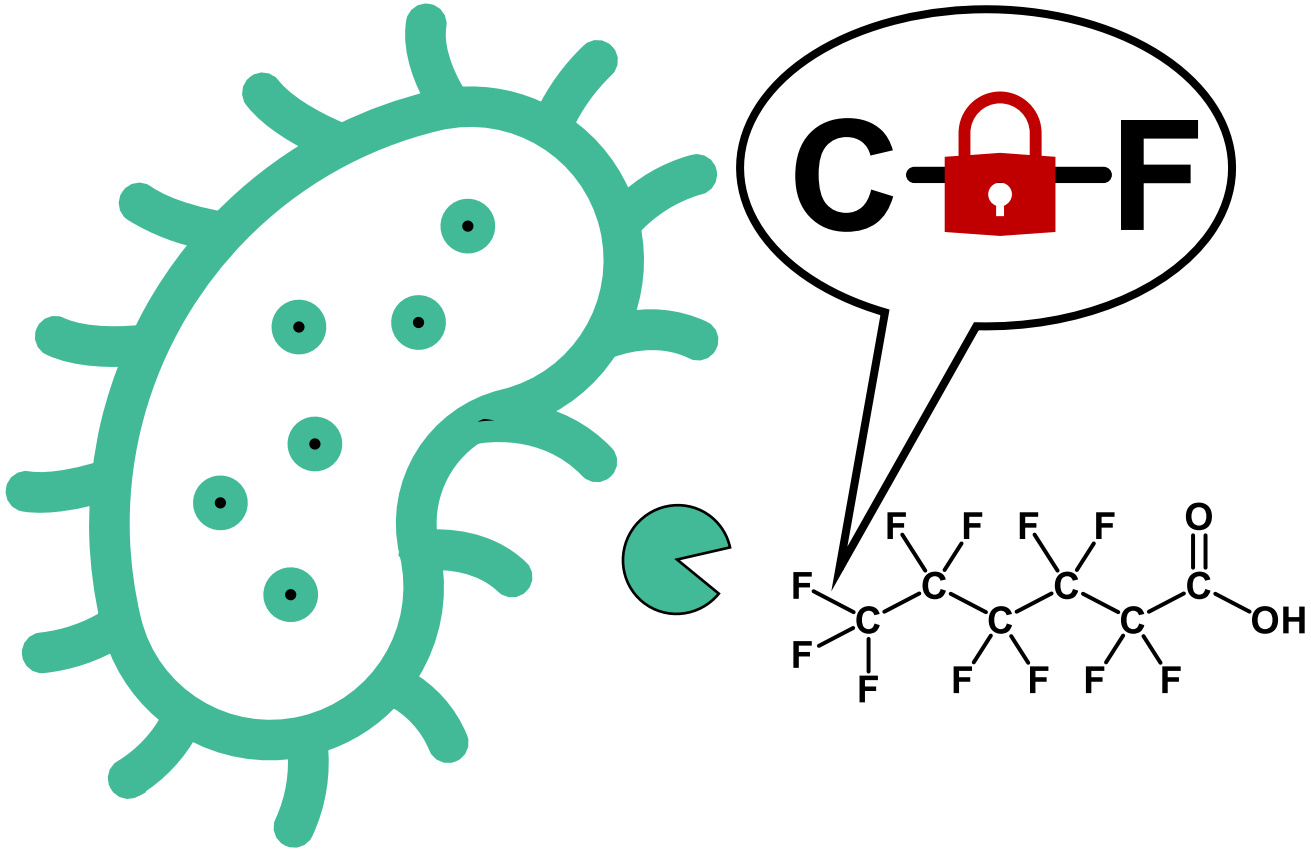
eawag aquatic research



The enviPath-PFAS biotransformation data package

May 11th 2025

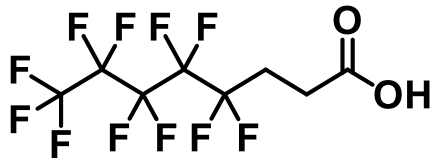
Per- and polyfluoroalkyl substances (PFASs) extremely persistent in the environment – DT_{50} ~ thousands of years



But! PFAS are diverse and contain "normal" organic functional groups as well

- Carboxylic acids
- Alcohols
- Sulfonamides
- Unsubstituted alkyl chains

Some polyfluorinated PFAS with these functional groups *can* be biotransformed in the environment posing a tricky situation for regulators…



"biodegradable"

Researchers are currently studying the ways in which polyfluorinated precursors can form perfluorinated end products

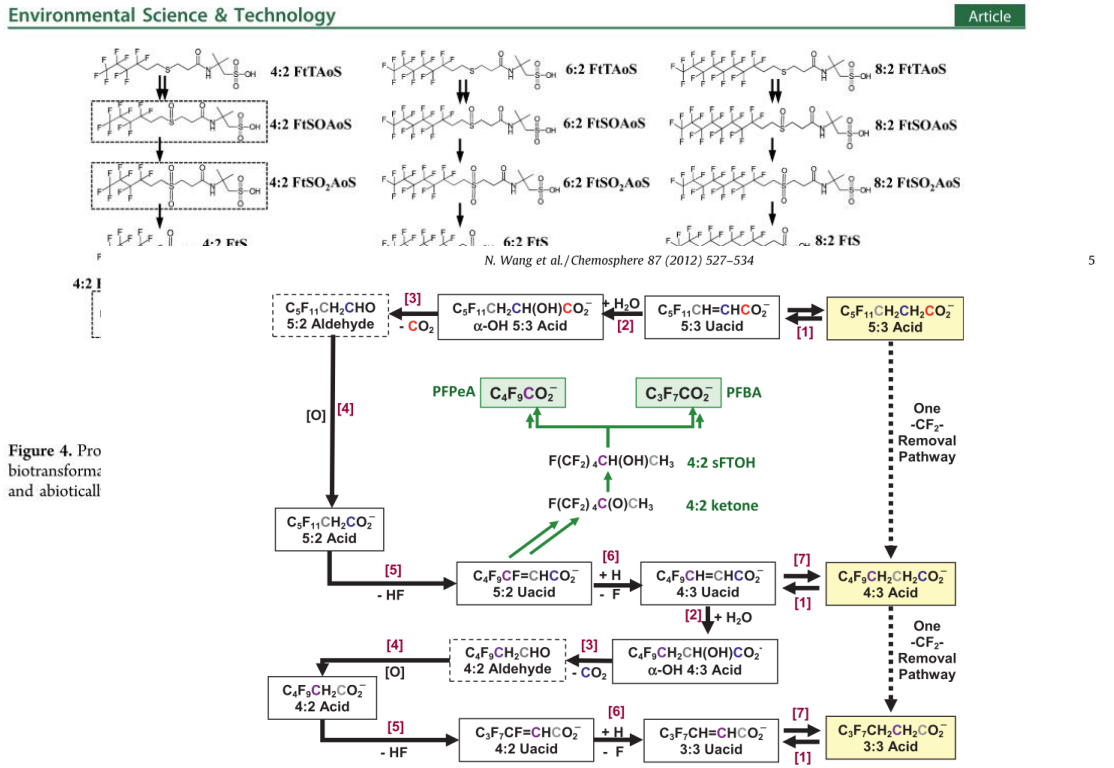


Figure 4. Pro
biotransforma
and abioticall

Fig. 5. Proposed 5:3 acid aerobic biotransformation pathways. The double arrows indicate multiple transformation steps. The bold black arrows indicate the "one-carbon removal pathways" for 5:3 acid to be converted to 4:3 acid. The green arrows indicate pathways leading to perfluorocarboxylates. The intermediate inside the dashed rectangular box is an expected transformation product. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

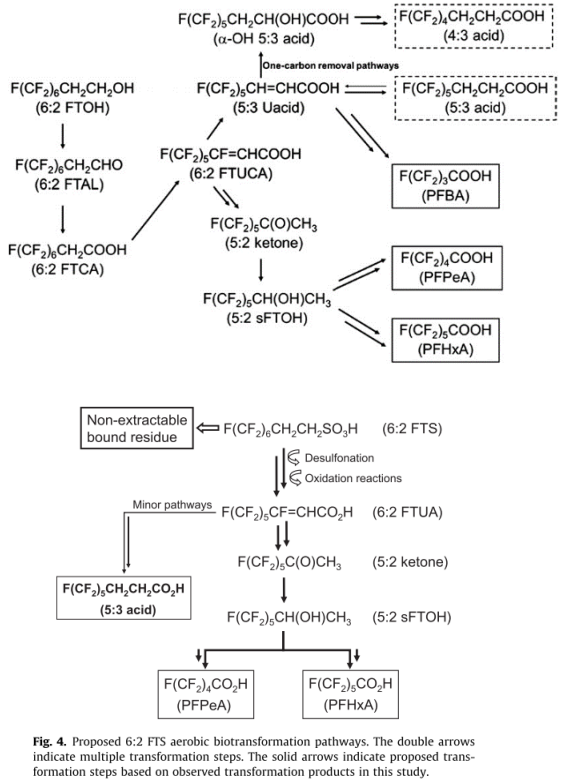
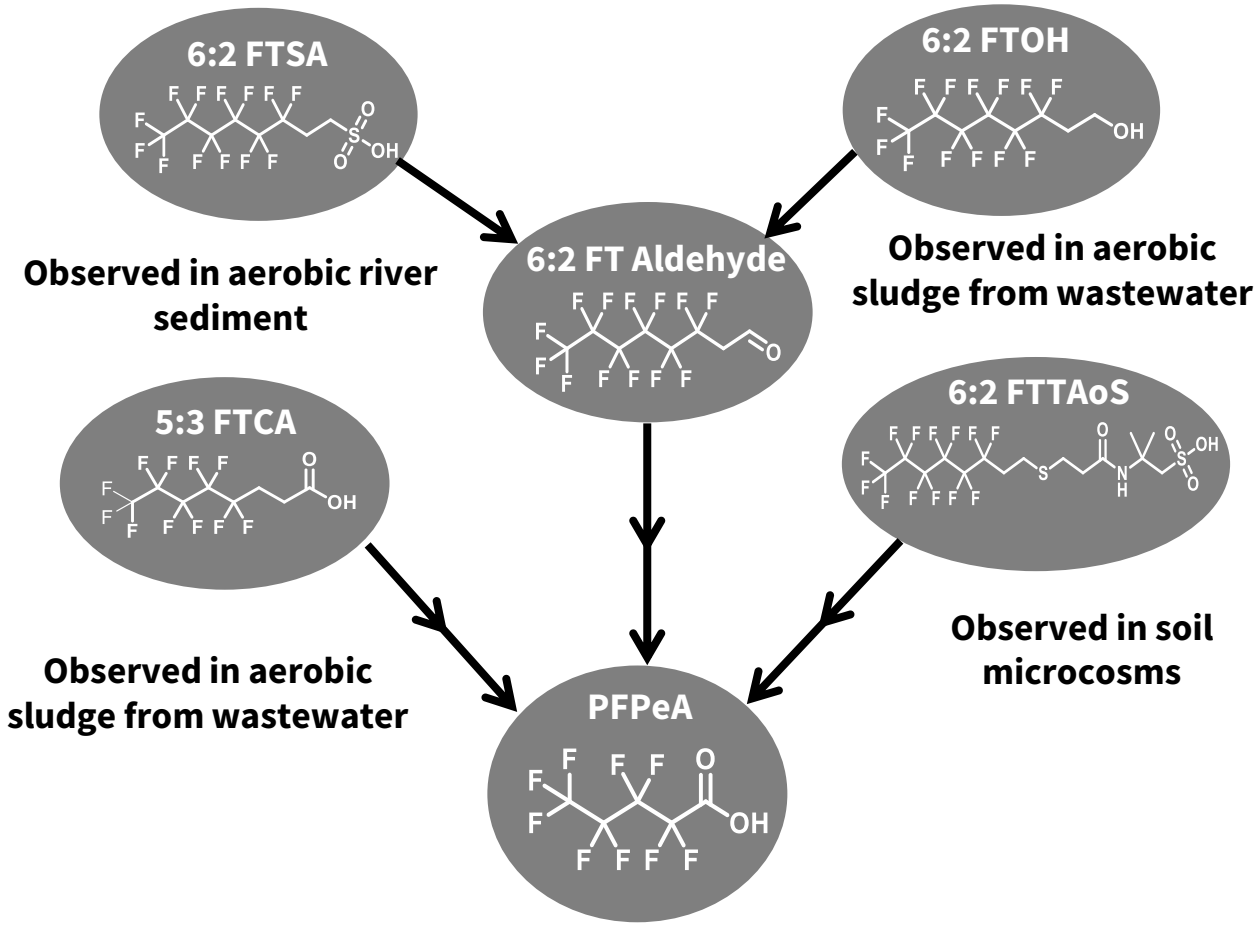


Fig. 4. Proposed 6:2 FTS aerobic biotransformation pathways. The double arrows indicate multiple transformation steps. The solid arrows indicate proposed transformation steps based on observed transformation products in this study.

We have been working to upload this data into the enviPath database

Harding-Marjanovic, K. C. *et al*. Aerobic Biotransformation of Fluorotelomer Thioether Amido Sulfonate (Lodyne) in AFFF-Amended Microcosms. *Env. Sci. Tech.* **49**, 7666-7674 (2015).
Wang, N. *et al.* 6:2 Fluorotelomer sulfonate aerobic biotransformation in activated sludge of wastewater treatment plants. *Chemosphere.* **82**, 853-858 (2011).
Wang, N. *et al.* 5:3 Polyfluorinated acid aerobic biotransformation in activated sludge via novel "one-carbon removal pathways". *Chemosphere.* **87**, 527-534 (2012).
Zhao, L. *et al*. 6:2 Fluorotelomer alcohol biotransformation in an aerobic river sediment system. *Chemosphere.* **90**, 203-209 (2013).

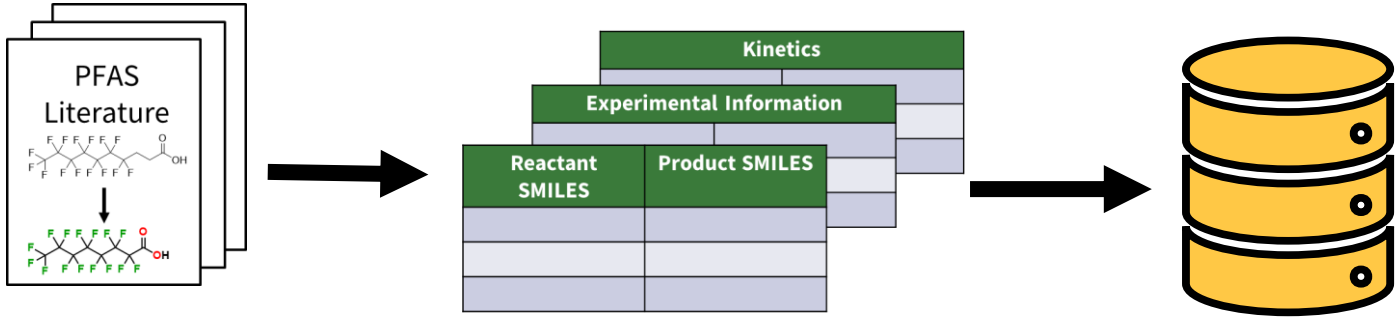
We especially need to synthesize data for PFASs given their extreme persistence and toxicity

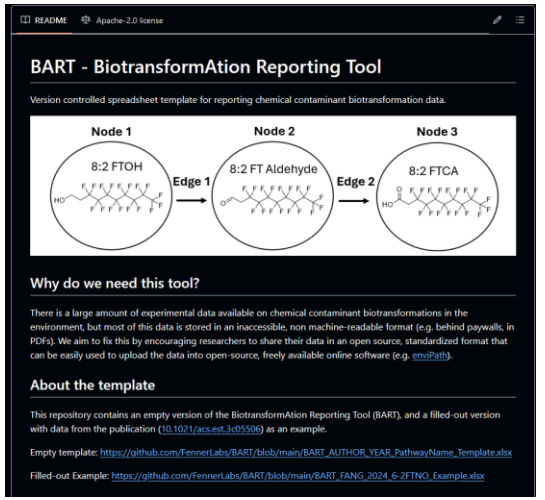


Many polyfluorinated precursors form similar perfluorinated end products, even in different environmental compartments

This again poses a challenge for regulators seeking who to blame for contaminated sites

We have translated PFAS biotransformation data from literature into an enviPath-PFAS package





We currently have information from 35 papers in the database

We know of 110 papers containing PFAS biotransformation data and are working to add all information available

Biotransformation Reporting Tool (BART)

What is available in the enviPath-PFAS package?

Home / Package / enviPath-PFAS

enviPath-PFAS

Actions

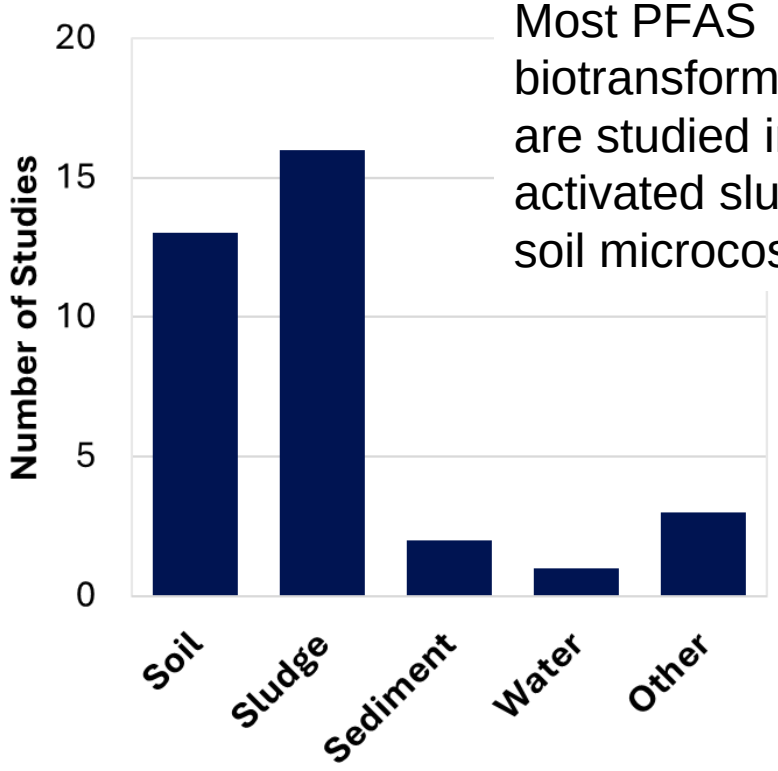
First public version of the enviPath-PFAS package. Created on April 22nd 2025.

Pathways	71
Rules	0
Compounds	316
Reactions	545
Relative Reasoning	0
Scenarios	530

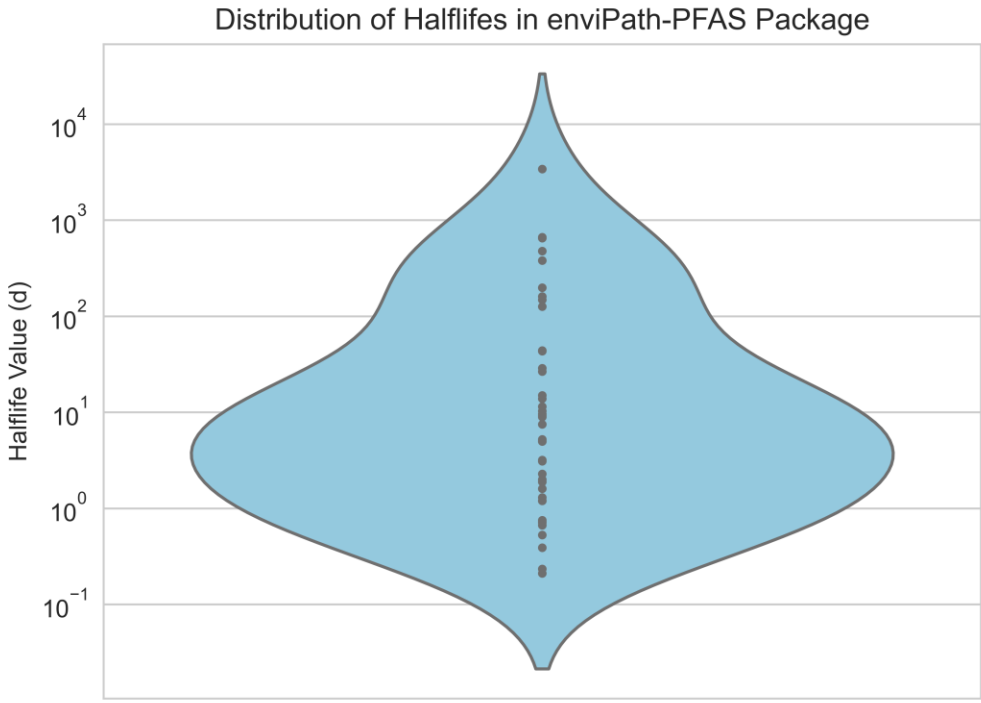
enviPath-PFAS Package

Note: if you know of an important PFAS biotransformation pathway, and do not see it in the package, please let us know!

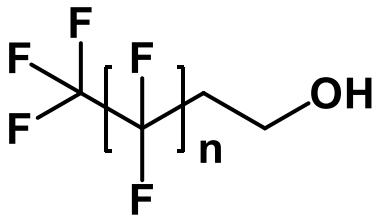
Data available in the enviPath-PFAS package so far



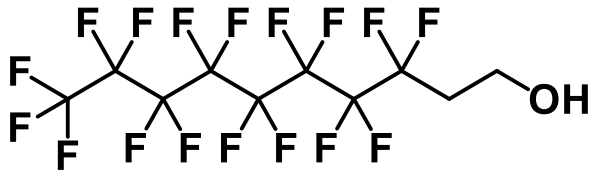
Most PFAS biotransformations are studied in activated sludge or soil microcosms



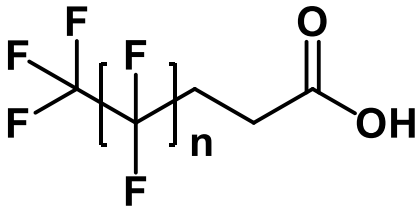
Many experimental studies test PFAS with similar head groups and different carbon chain lengths



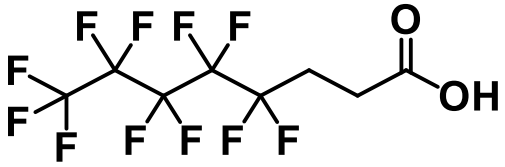
Fluorotelomer Alcohols
(10 pathways)



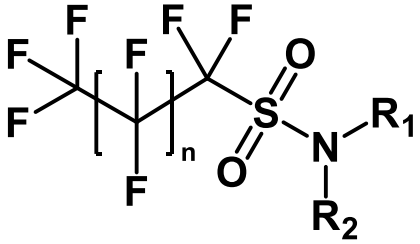
8:2 Fluorotelomer Alcohol



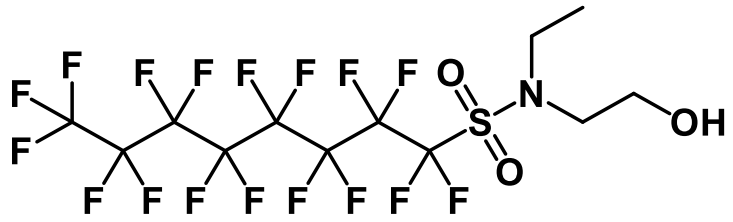
Fluorotelomer Carboxylic Acids
(8 pathways)



5:3 Fluorotelomer Carboxylic Acid

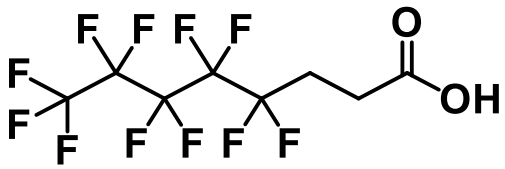


Perfluoroalkyl sulfonamides
(11 pathways)



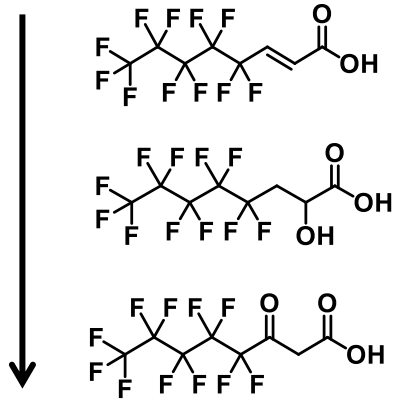
N-Ethyl Perfluorooctanesulfonamidoethanol (N-EtFOSE)

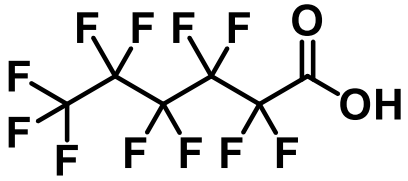
Commonly observed PFAS biotransformations - FTCAs



5:3 Fluorotelomer Carboxylic Acid

"β-oxidation-like" pathway





Perfluorohexanoic Acid

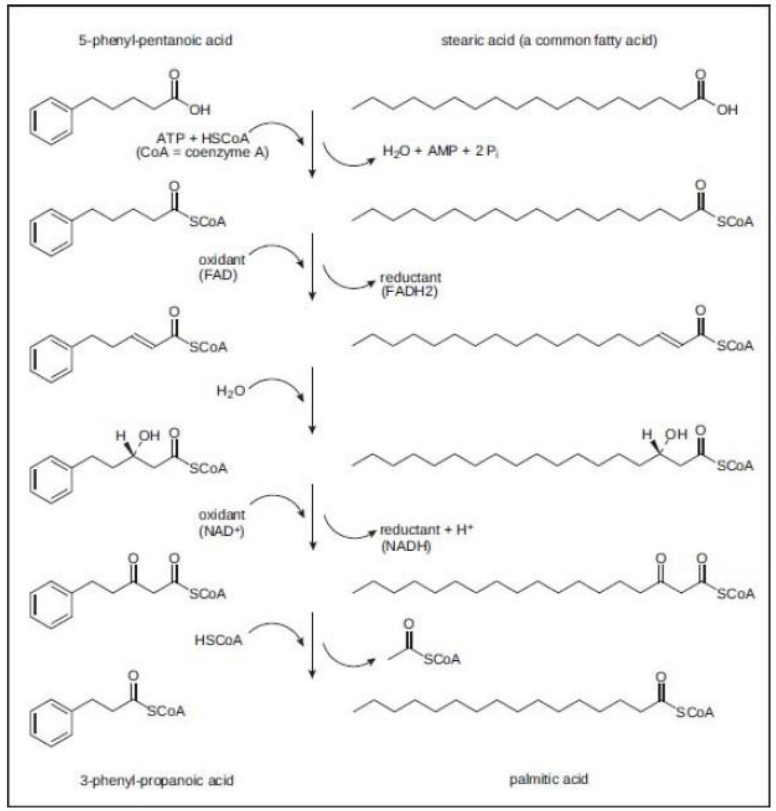
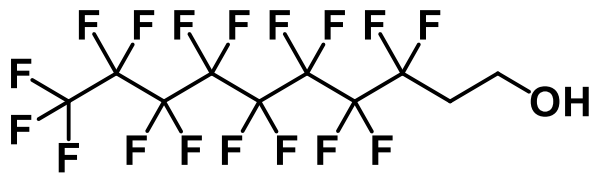


Figure 26.2 Parallel "beta oxidation" pathways for a xenobiotic substituted benzene, 5-phenyl pentanoic acid, and a naturally occurring fatty acid, stearic acid (Nelson and Cox, 2000).

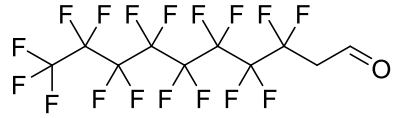
Geng, F. & Helbling, DE. Cascading Pathways Regulate the Biotransformations of Eight Fluorotelomer Acids Performed by Wastewater Microbial Communities. *Env. Sci. Tech.* **58**, 23201-23211 (2024).

Commonly observed PFAS biotransformations – n:2 FTOHs

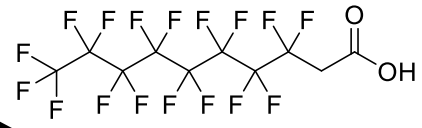


8:2 Fluorotelomer Alcohol

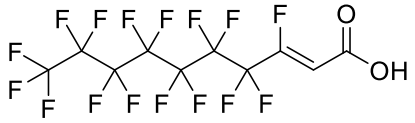
Aldehyde



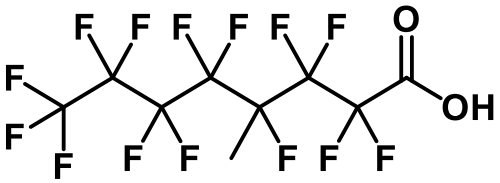
Carboxylic Acid



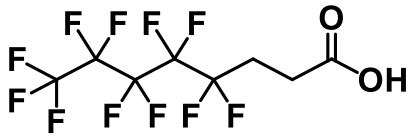
Unsaturated Carboxylic Acid



PFOA

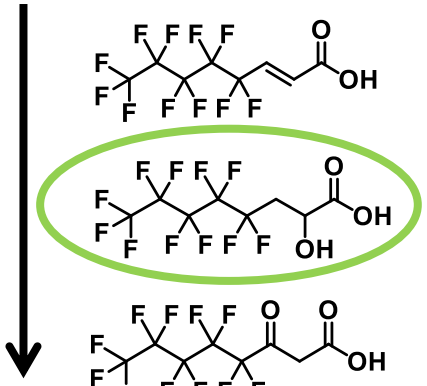


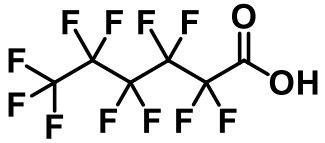
Current pathway prediction models in enviPath do not provide many useful transformation products for PFASs



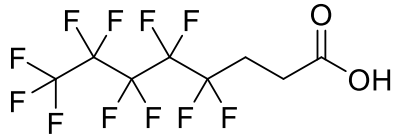
5:3 FTCA

Experimentally Observed Pathway





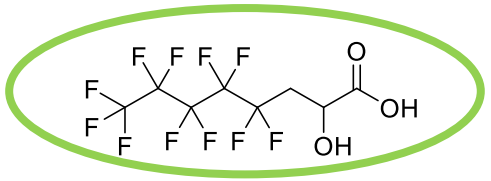
PFHxA



5:3 FTCA

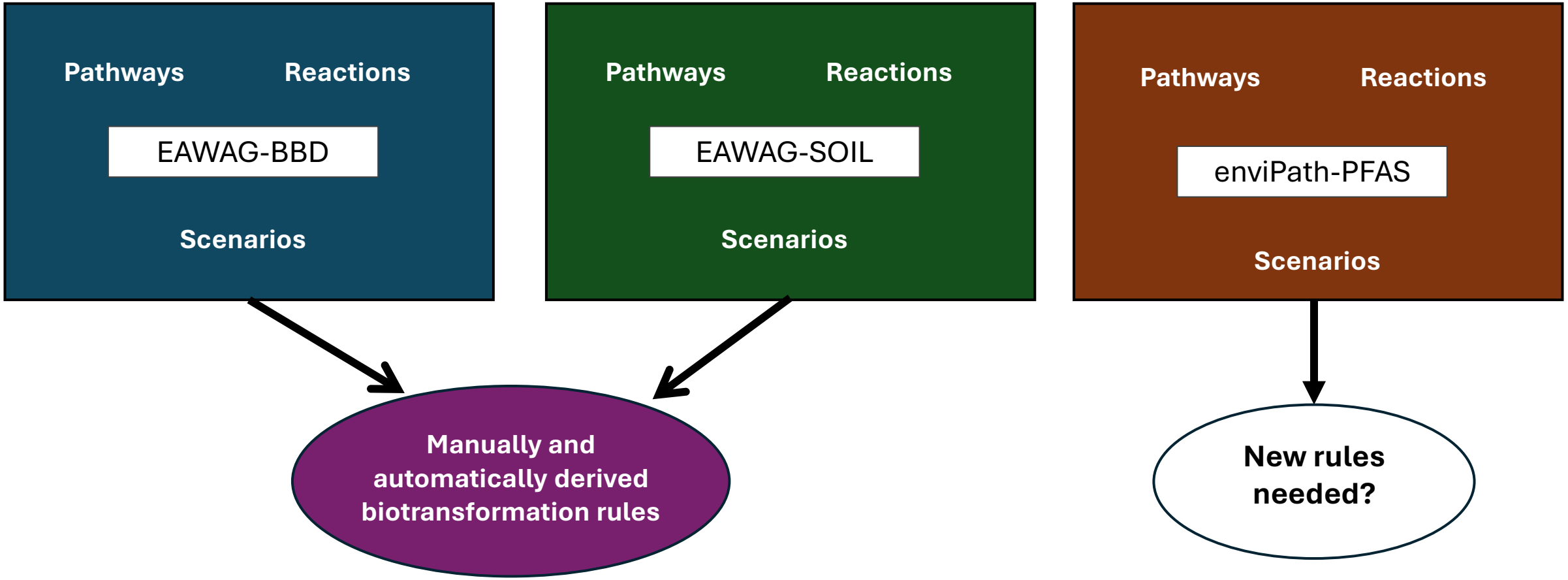
Pathway predicted using default prediction model (threshold = 0.5)

bt0242 (hydroxylation of unsubstituted carbon chain)

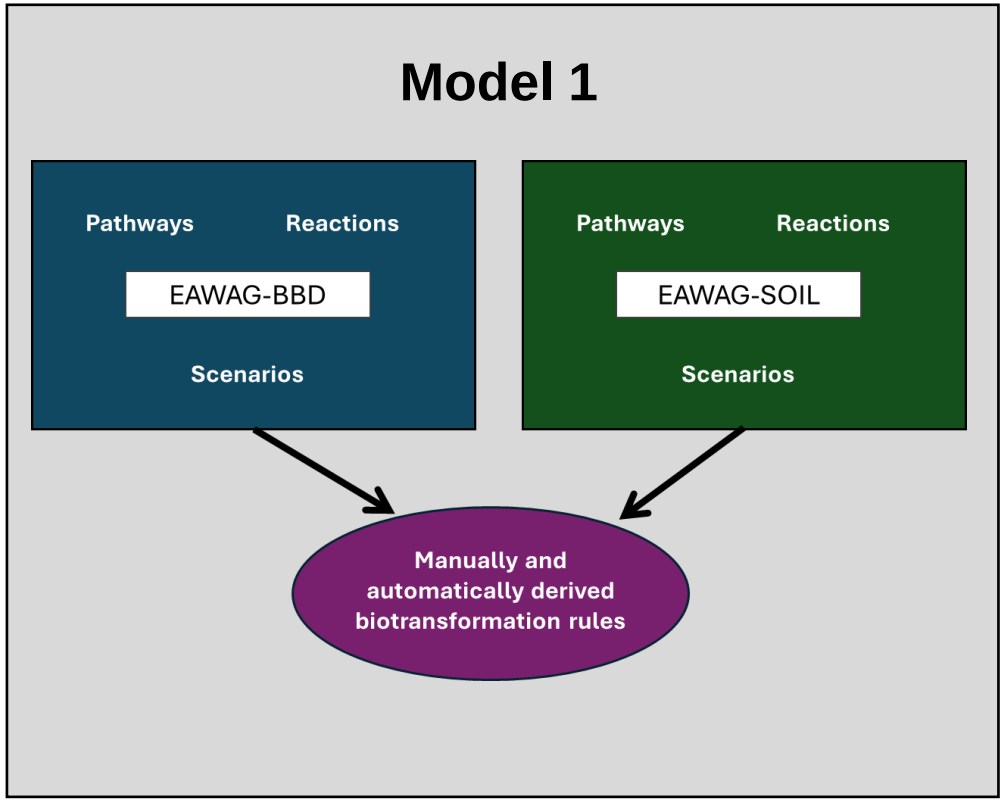


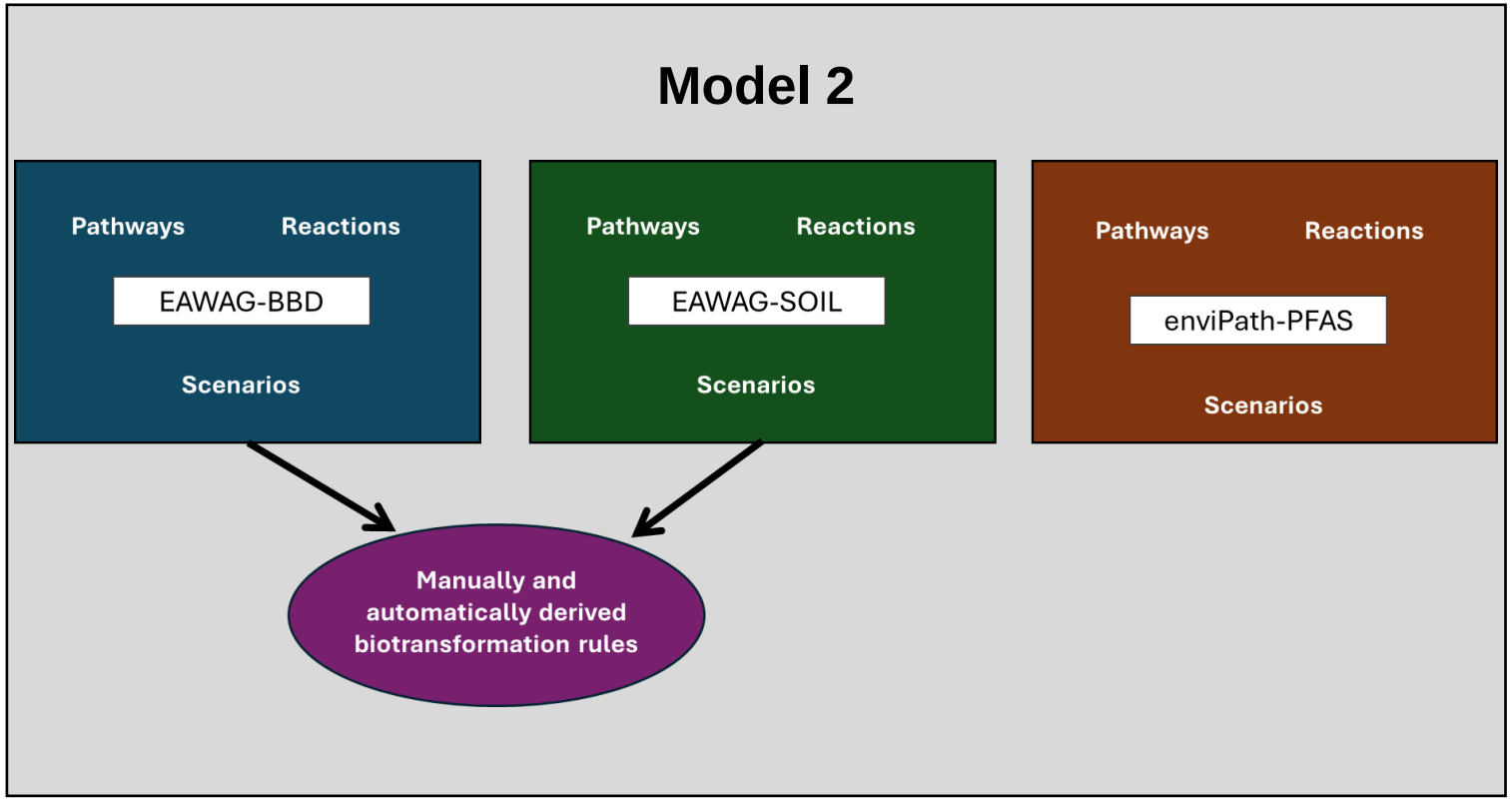
Hydroxylated intermediate

We are using data in the enviPath-PFAS package to help improve pathway predictions for PFAS

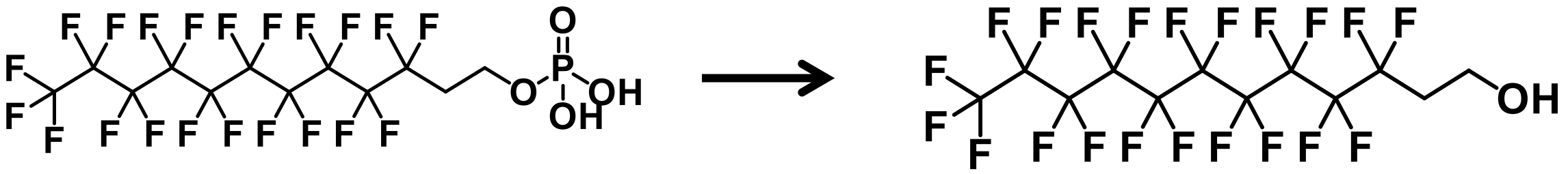


We have started training a pathway prediction model with the enviPath-PFAS data included





We tested the model predictions for one simple pathway



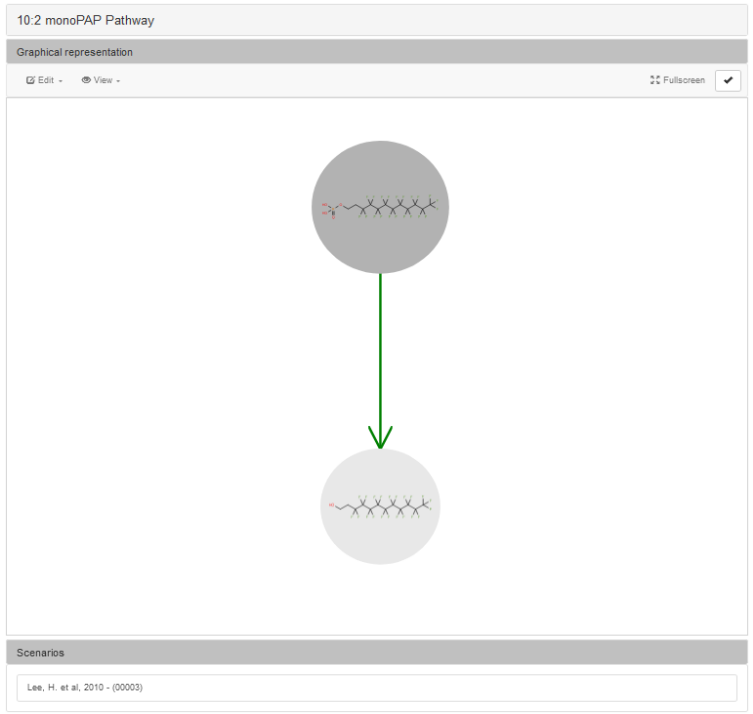
10:2 monoPAP

10:2 FTOH

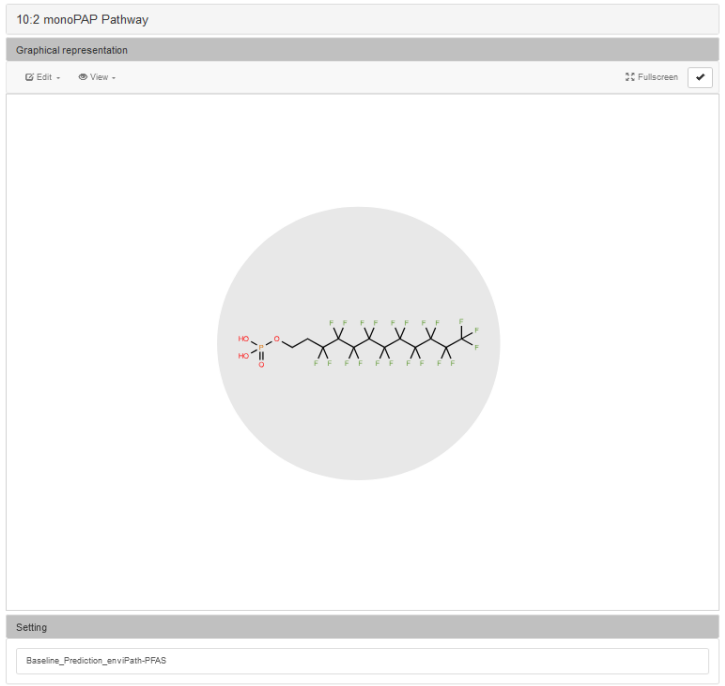
Lee, H. *et al*. Biodegradation of Polyfluoroalkyl Phosphates as a Source of Perfluorinated Acids to the Environment. *Env. Sci. Tech.* **44**, 3305-3310 (2010).

The pathway with PFAS training data generated better predictions

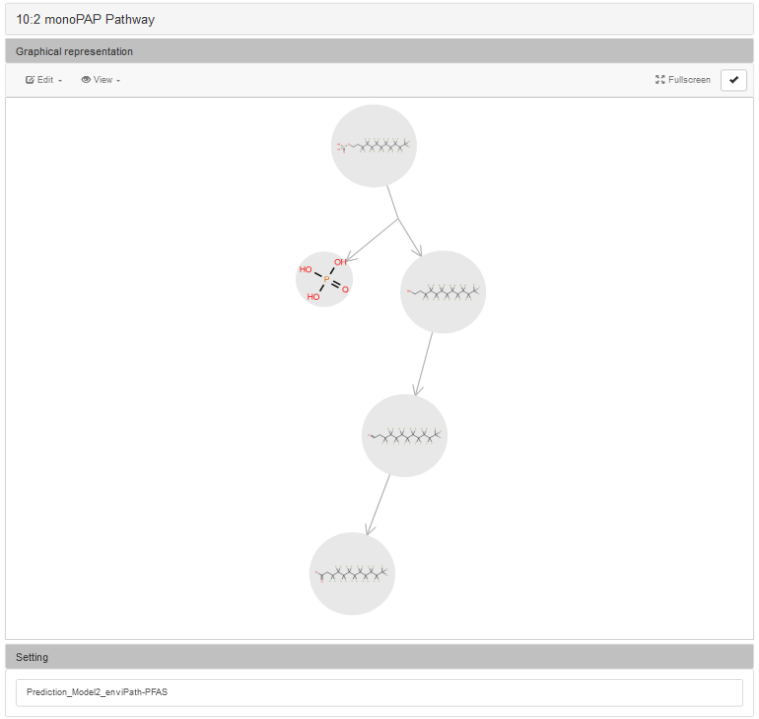
Actual (reported) pathway



Model 1

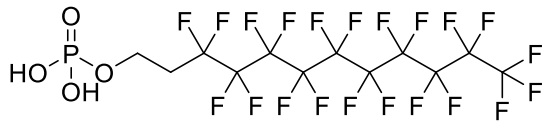


Model 2

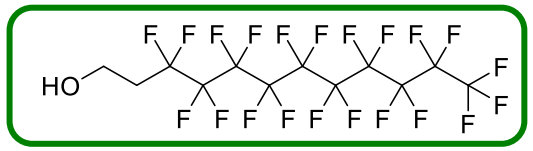


Model 2 even predicted likely biotransformation products beyond what was reported

Actual (reported) pathway

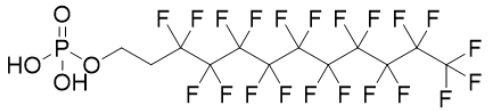


10:2 monoPAP

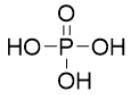


10:2 FTOH

Model 2 Predicted

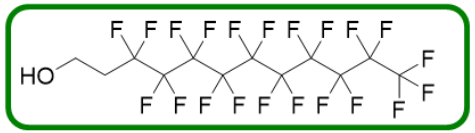


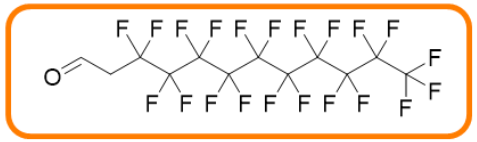
10:2 monoPAP



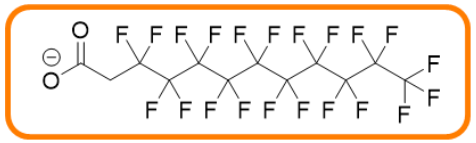
Phosphate

10:2 FTOH





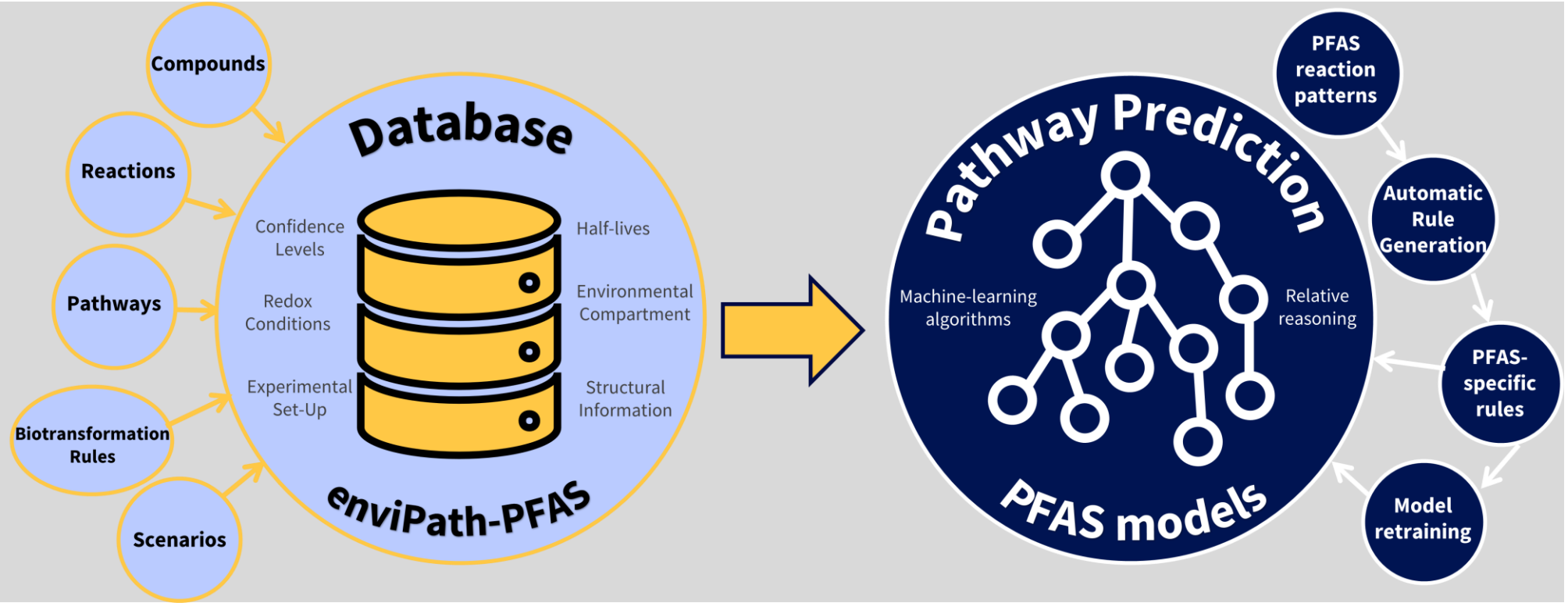
10:2 FT Aldehyde



10:2 FTCA

Outlook for the enviPath-PFAS package

1. We need more data!
2. New pathway prediction models will be trained with PFAS biotransformation data
3. There are likely new PFAS-specific biotransformation rules that need to be implemented into prediction models



enviPath-PFAS Package

Acknowledgements

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