Contaminant biotransformation pathways and kinetics

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The enviPath database, Open Research Data, and prediction tools

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Universität Zürich[UZH]

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Workshop schedule

Morning schedule

Time	Topic	Presenter
08:30 – 08:45	Introduction	Kathrin Fenner
08:45 – 09:30	Fundamentals of biodegradation and biodegradation modeling	Kathrin Fenner
09:30 – 10:00	Elements of biodegradation data & data packages in enviPath	Jasmin Hafner
10:00 – 10:30	Uploading, sharing and extracting biotransformation data in enviPath	Stephanie Rich
10:30 – 11:00	***Health break (Catering: 10:30 – 10:45)***	
11:00 – 11:30	Introduction to predictive models in enviPath	Jörg Wicker
11:30 – 12:00	Hands-on exercises in predictive modeling	Jörg Wicker, Tim Lorsbach
12:00 – 13:30	***Lunch break (Catering: 12:30 – 13:30)***	

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Workshop schedule

Afternoon schedule

Time	Topic	Presenter
13:30 – 14.00	Generating suspect lists for transformation product screening	Athira Shankar
14:00 – 14:30	Pathway data in industrial R&D	Sebastian Schmidt
14:30 – 15:00	PFAS biotransformation data package	Stephanie Rich
15:00 – 15:30	***Health Break (Catering: 15:15 – 15:30)***	
15:30 – 16:00	Linking enviPath to systems biology and sequencing data	Jasmin Hafner
16:00 – 16:30	Ongoing developments of enviPath: Applicability domain, evaluation, transformers	Jörg Wicker
16:30 – 17:00	PEPPER predicts persistence and facilitates developing new models	José Cordero

Workshop materials

All workshop slides can be found at the enviPath community site:

https://community.envipath.org/t/setac-2025-vienna-workshop/53

Short introduction round

1. My knowledge about biotransformation of chemicals is advanced / intermediate / beginner's level
2. My background is in academic research / industry research / others
3. I have used biotransformation predictions tools before (Y/N, which)
4. What would you like to learn today?