April 15, 2025

Hands-on exercises in predictive modeling

Jörg Simon Wicker Tim Lorsbach
enviPath / School of Computer Science – University of Auckland

enviPath

UNIVERSITY OF AUCKLAND
Waipapa Taumata Rau
NEW ZEALAND

SCIENCE

Predicting Biodegradation Pathways

- The goal of this session is to use enviPath to predict a biodegradation pathway
- We will pick a compound then use the enviPath web interface to predict its metabolic fate

Pick a compound!

- First, pick your favourite compound and get the SMILES string for it
- Or use Spiroxamine: CCCN(CC)CC1COC2(O1)CCC(CC2)C(C)(C)C

- Or caffeine: CN1C=NC2=C1C(=O)N(C)C(=O)N2C

Enter SMILES into enviPath prediction

- Got to `https://envipath.org`

- Enter the SMILES into the text field and click “Go”

Wait for results...

- You are now on the results page
- As long as the benzene ring on the right top is spinning, the prediction is still running

- Reload the pathway once new metabolites are predicted (see the popup message)
  - When reloading you might get a pathway with compounds not connected to the rest, this means the pathway is predicted, but not fully written to the database yet, give it a few minutes and reload

Optional: modify pathway

- Sometimes, enviPath predicts compounds we are not interested in, for example formaldehyde
- If your predicted pathway has one of those unwanted compounds, you can remove it
  - Mark compound by clicking on it
  - Click Edit
  - Compound
  - Remove Compound only from this pathway
  - Delete

Examine the pathway

- Explore the pathway view, there is a lot of information in it
- Hover over the arrows / compounds, click on them
- What does it tell you about applicability domain?
- Can you find the probabilities for the reactions predicted by the models?

Advanced prediction

- Click “Pathway” or go to `https://envipath.org/pathway`

- Click “Actions” ⇒ “New Pathway”
- Try the incremental prediction
  - Chose the node to continue from, click it and click “predict from here”

Advanced: use the python interface

- Use our Python library at `https://github.com/enviPath/enviPath-python`

- Try the “Predict Patways” example!

enviPath

UNIVERSITY OF AUCKLAND
Waipapa Taumata Rau
NEW ZEALAND

SCIENCE

Thank you for listening! Any questions?

https://envipath.org
https://envipath.com