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Hands-on exercises in predictive modeling

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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!

EP



- 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://setac<1-10>.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



The screenshot shows a web interface for a chemical pathway prediction tool. At the top, there is a grey header with the text "Graphical representation". Below the header, there is a navigation bar with "Edit" and "View" options on the left, and "Fullscreen" and a spinning benzene ring icon on the right. The main content area displays a chemical structure of a complex molecule with a central benzene ring and several substituents. A notification popup is visible in the bottom right corner, containing the text "Pathway has been updated." and two buttons: "Reload" and "Hide".

- 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

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- 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”



Try our new model and updated implementation!

EP



- Go to <https://playground.envipath.org>
- Chose “Predict Pathway” ⇒ “Predict Pathway”
- Draw your compound or use Ctrl-C / Ctrl-V to paste a SMILES into the interactive field
- Click “Predict”
- Check the predicted pathway (and be amazed by the speed)
 - This uses our new purely data-driven enviFormer model



Advanced: use the python interface



- Use our Python library at
<https://github.com/enviPath/enviPath-python>
- Try the “Predict Patways” example!



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Thank you for listening! Any questions?

<https://envipath.org>

<https://envipath.com>