PEPPER Predicts Persistence and Facilitates Developing New Models

Presented by Jose Cordero

Collaborators: Jasmin Hafner & Kathrin Fenner

SETAC Europe - Workshop on Contaminant Biotransformation Pathways and Kinetics

Vienna, May 2025

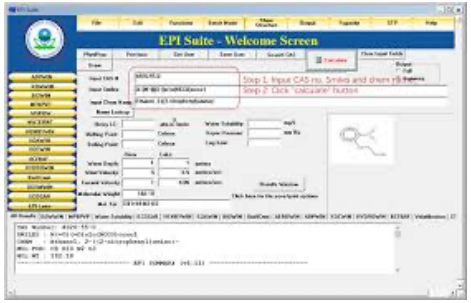
Predicting persistence remains elusive

We all want to predict persistence but there is no clear solution

Some examples:

OPERA
OPEn (q)saR App

VEGA



The the main objective of these tools is not persistence

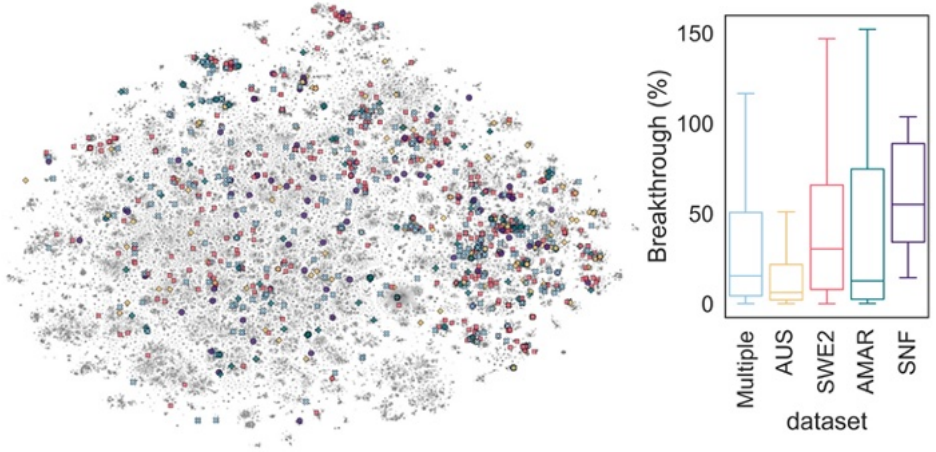
They rely heavily on BIOWIN

Not everything is open source

PEPPER models use the latest data

Our models are built using high quality experimental data

Fully transparent code and large training sets

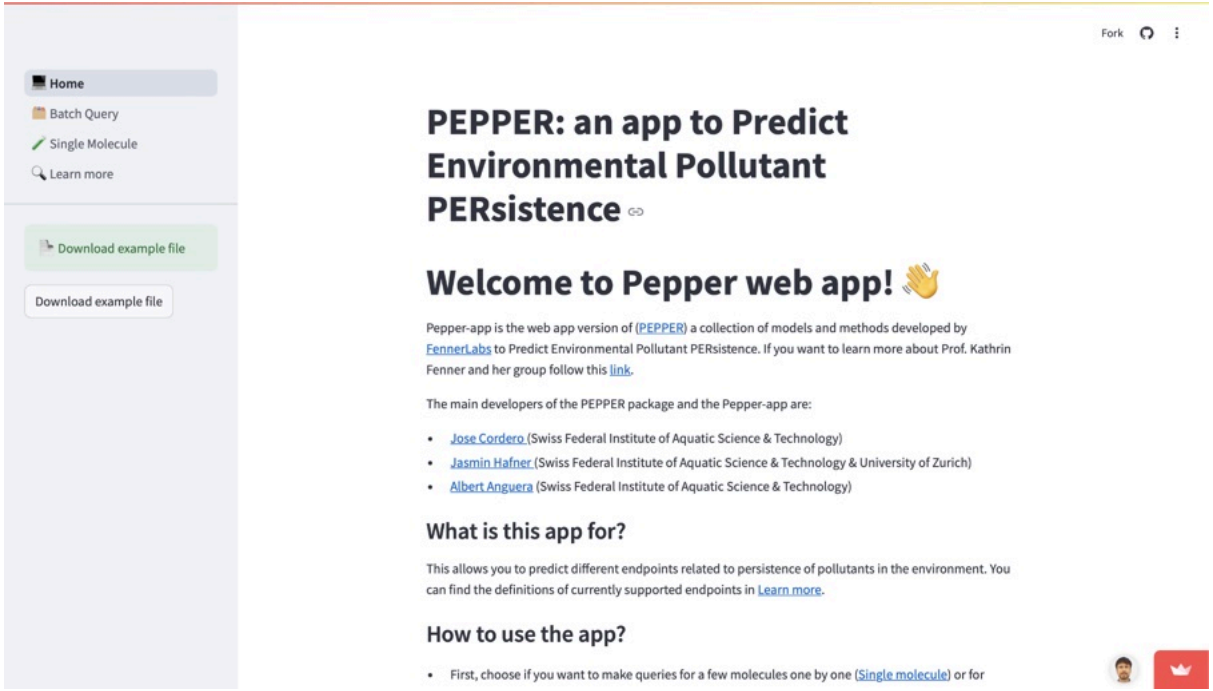


Check our talks on Wednesday for more information

How are PEPPER models available?

pepper-app is a web app

pepper-app only requires a list of SMILES



This month we added two DT50 models

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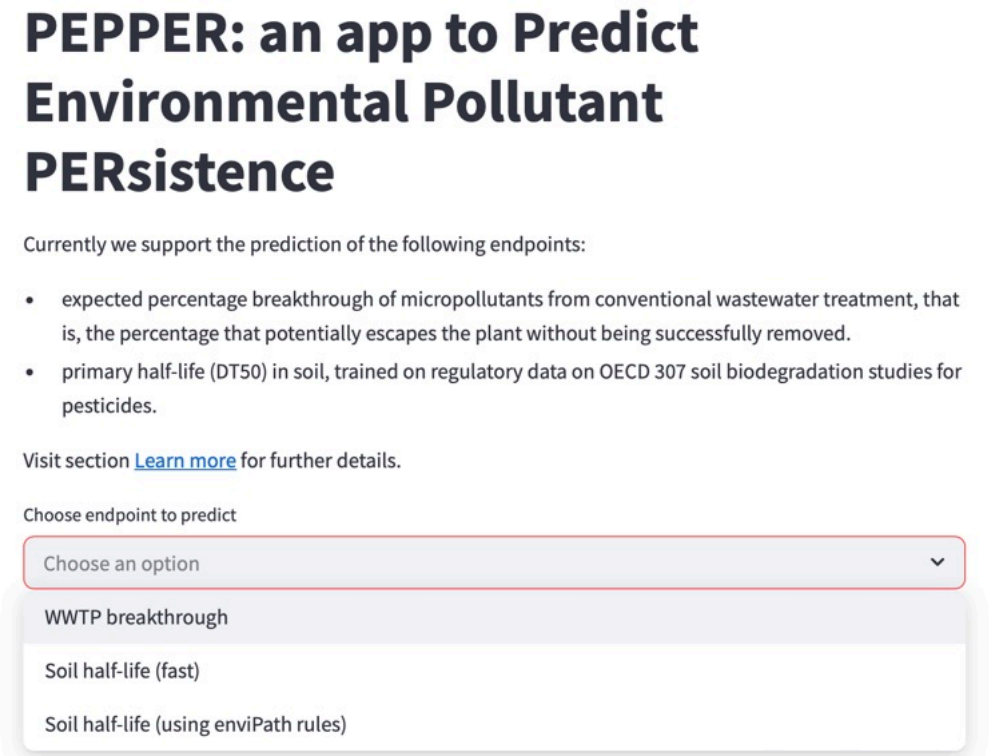

Predictions: endpoint + confidence metric

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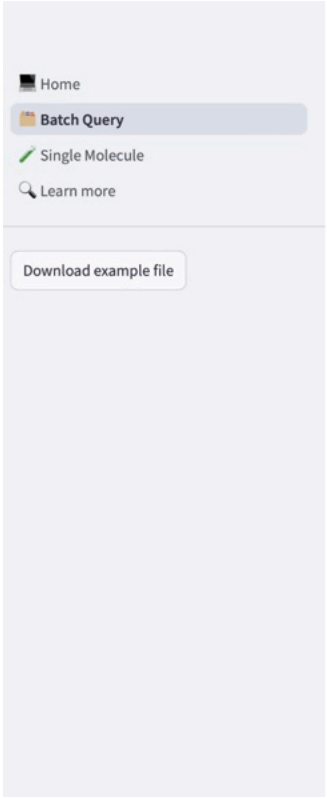
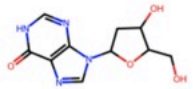
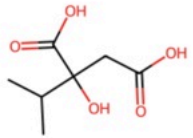
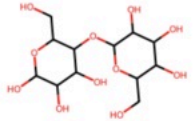


Sha

	Name	Breakthrough (%)	Confidence 0-1	Structure
0	2'-Deoxyinosine	3.4	0.54	
1	2-Isopropylmalic acid	6.7	0.56	
2	alpha-Lactose	28.3	0.36	

Also available as a docker + *rough* API

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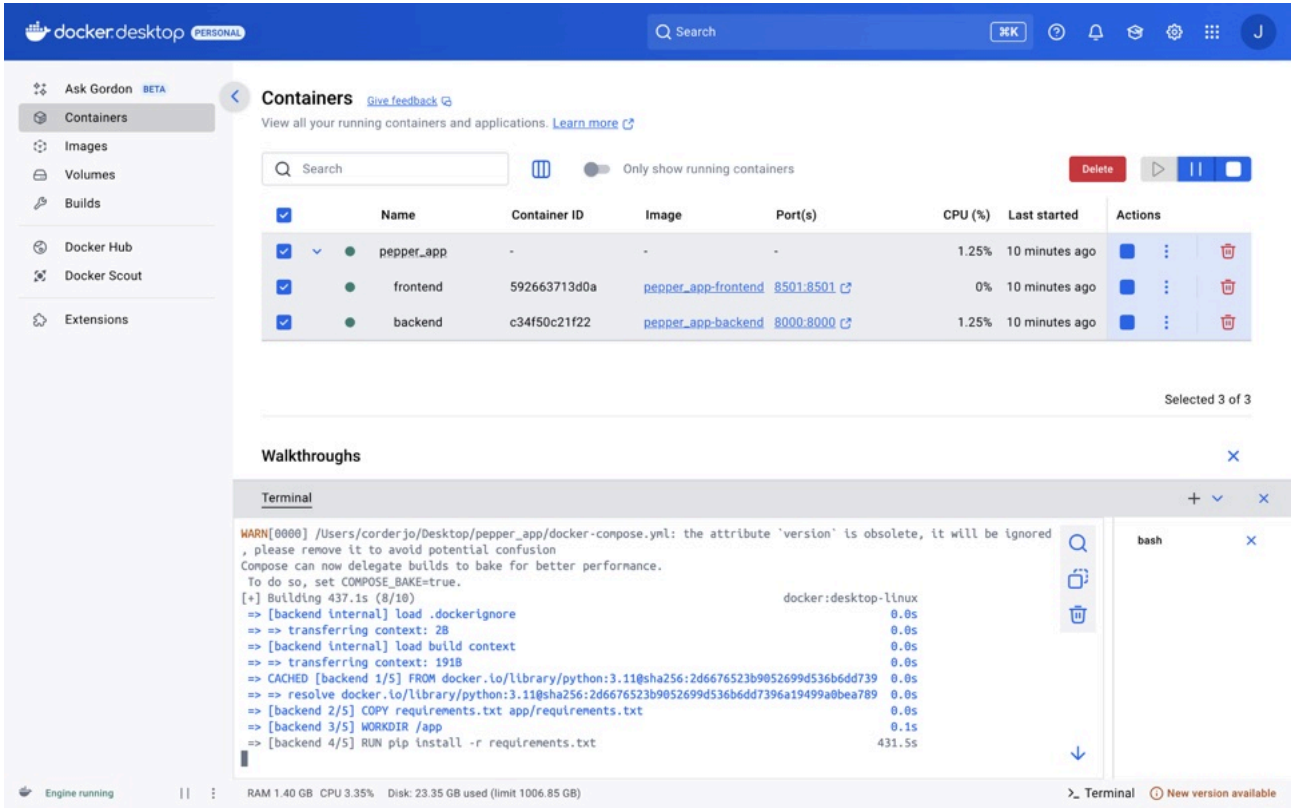

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Can I still see the models & scripts?

pepper-lab includes all code & methods

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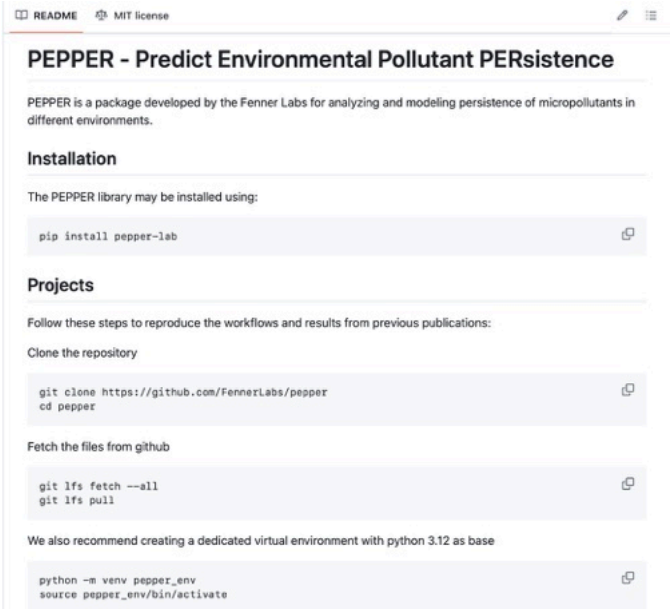
Github

https://github.com/FennerLabs/pepper


README MIT license

PEPPER - Predict Environmental Pollutant PERsistence

PEPPER is a package developed by the Fenner Labs for analyzing and modeling persistence of micropollutants in different environments.

Installation

The PEPPER library may be installed using:

```
pip install pepper-lab
```

Projects

Follow these steps to reproduce the workflows and results from previous publications:

Clone the repository

```
git clone https://github.com/FennerLabs/pepper
cd pepper
```

Fetch the files from github

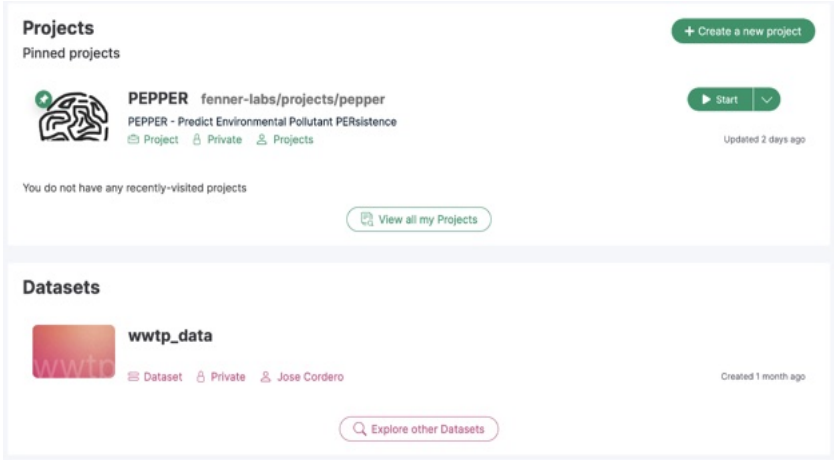
```
git lfs fetch --all
git lfs pull
```

We also recommend creating a dedicated virtual environment with python 3.12 as base

```
python -m venv pepper_env
source pepper_env/bin/activate
```

RENKU is a Swiss initiative linked to Gitlab

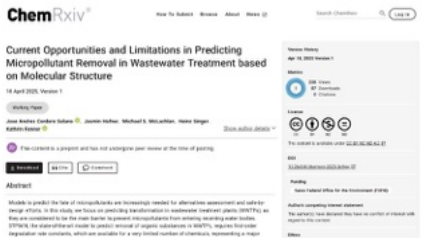
https://gitlab.renkulab.io/fenner-labs/projects/pepper



Details of models have been published

Available publications:

https://pubs.acs.org/doi/full/10.1021/acs.estlett.3c00526



https://chemrxiv.org/engage/chemrxiv/article-details/6800a831e561f77ed46c22b9

Soil models manuscript in preparation

Talks in SETAC:

Wednesday 10 am:

Hafner

3.10.A.T-03

Wednesday 3:15 pm:

Cordero

3.05.T-04

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You said “facilitates developing”...

Modules of the package

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Data Processing

Calculating Descriptors

Building & Validating Models

Predicting

Retraining or developing new models

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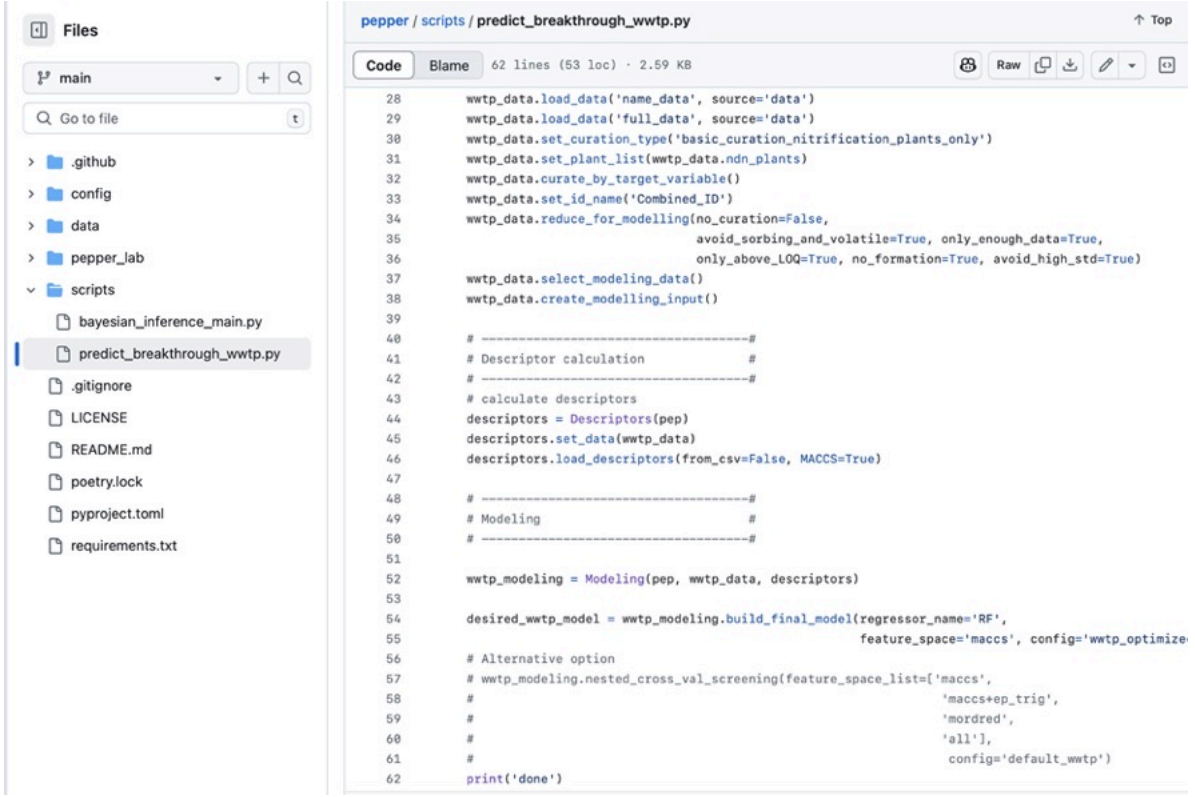

Acknowledgements

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