OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE

ModelRX

Modelling for Prediction or Read Across

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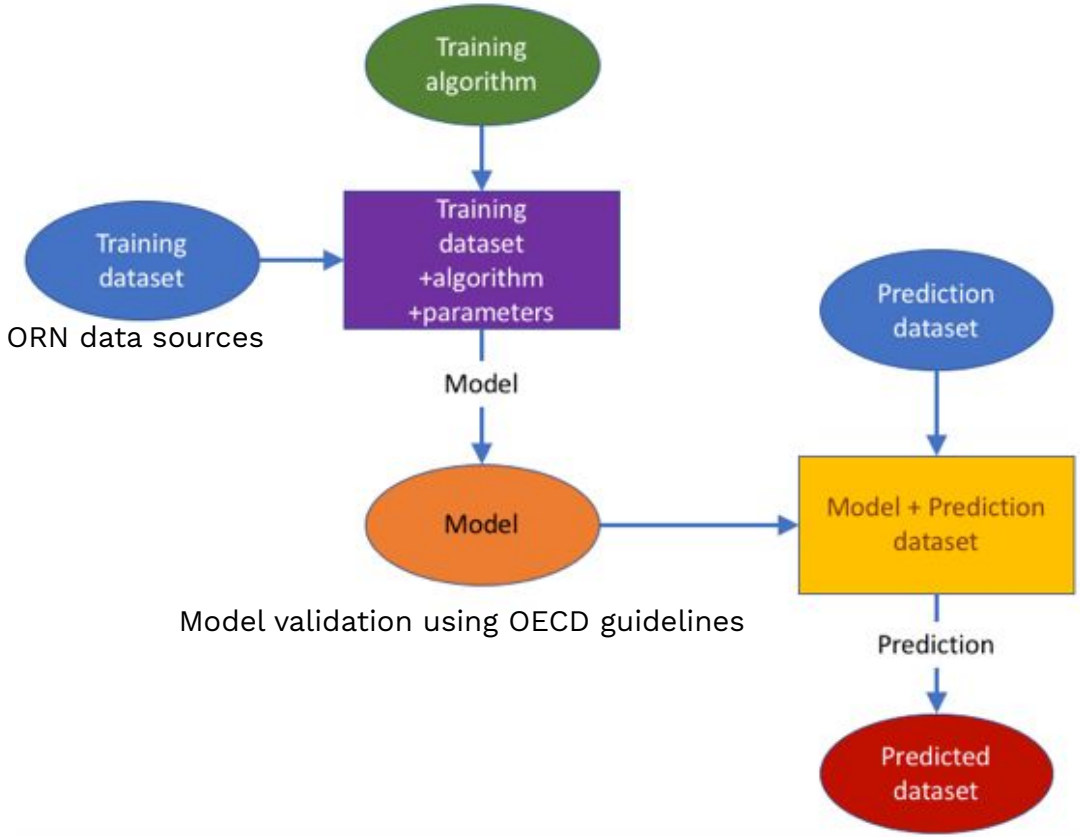
NTUA, UU, JGU/IST

OpenRiskNet: Open e-Infrastructure to Support Data Sharing, Knowledge Integration and *in silico* Analysis and Modelling in Risk Assessment
Project Number 731075

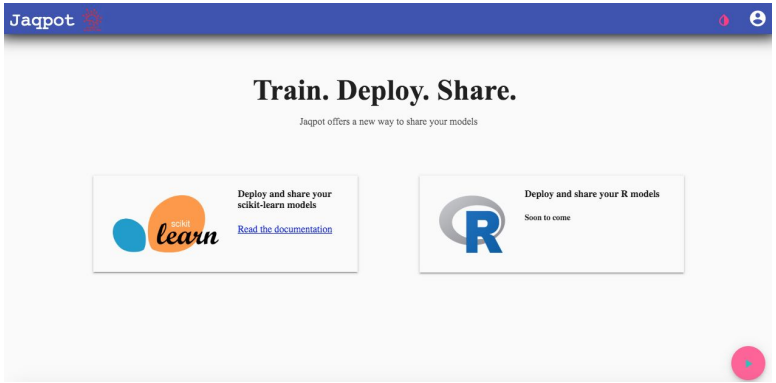
Case Study objective

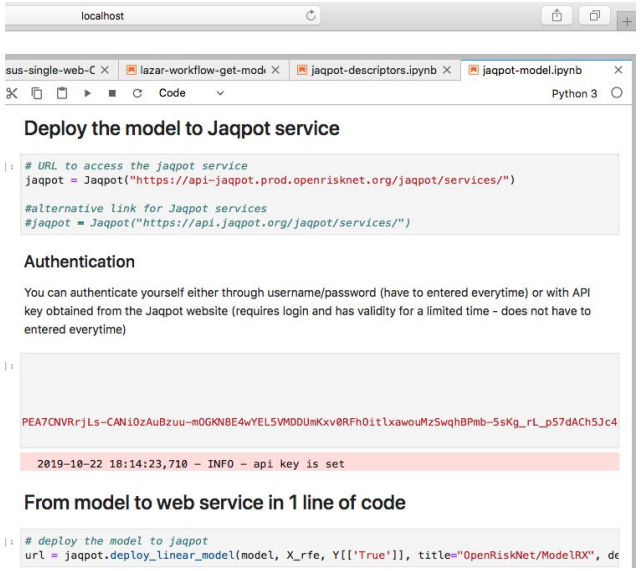
- support **similarity identification** in the DataCure case study (tools to calculate theoretical descriptors of substances)
- **fill gaps** in incomplete datasets
- use in-silico **predictive modelling approaches** (read-across, QSAR) to support final risk assessment

Workflow for prediction model



Jaqpot (NTUA)



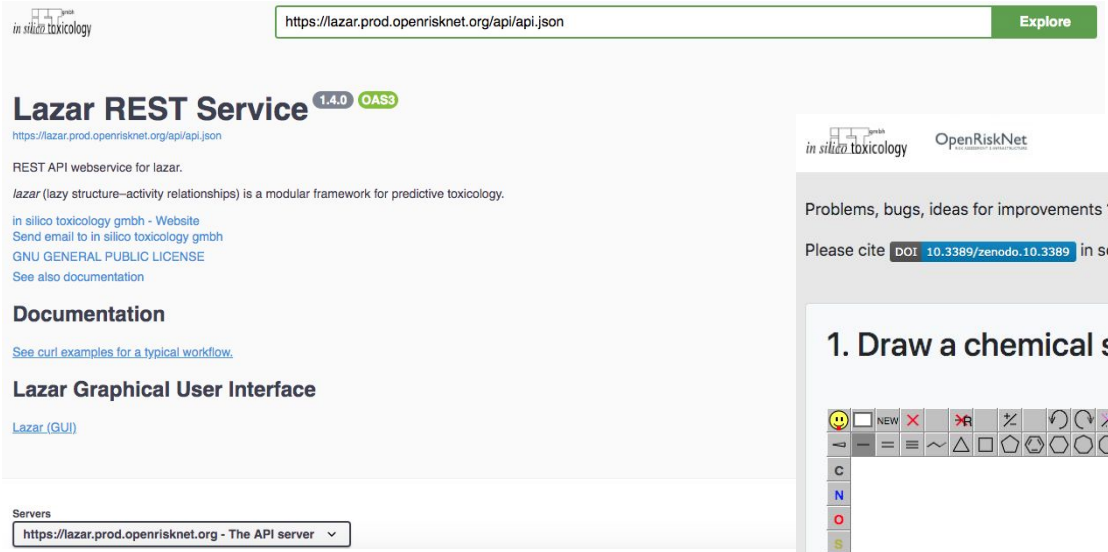


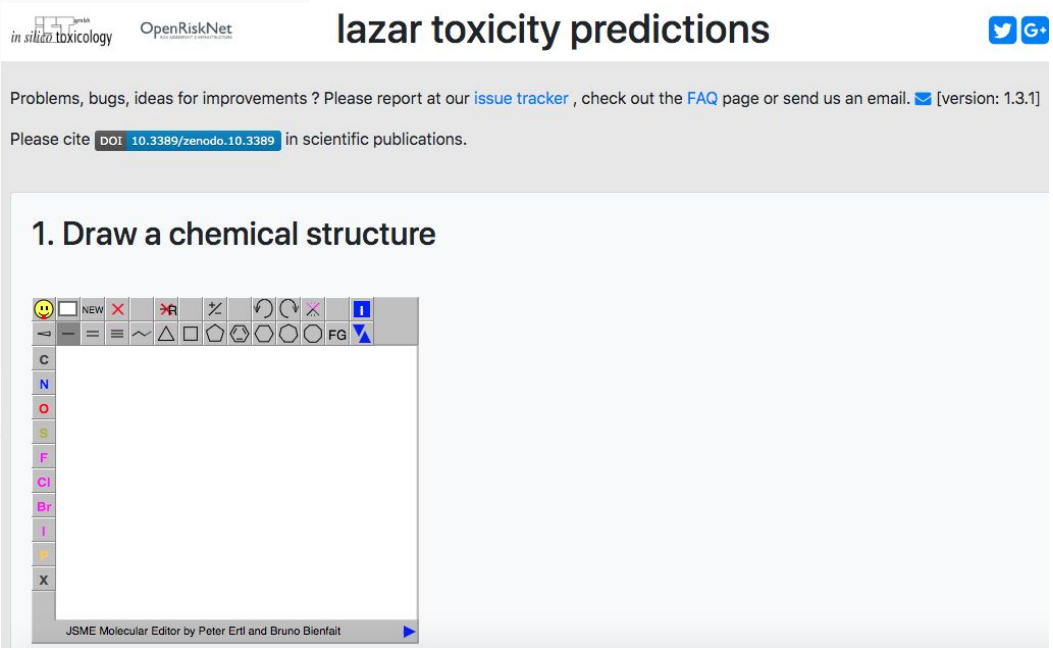
modelling and analysis services

- scaling
- normalisation
- variable selection
- model validation
- algorithms for DoA
- QMRF reports

Lazar (JGU)

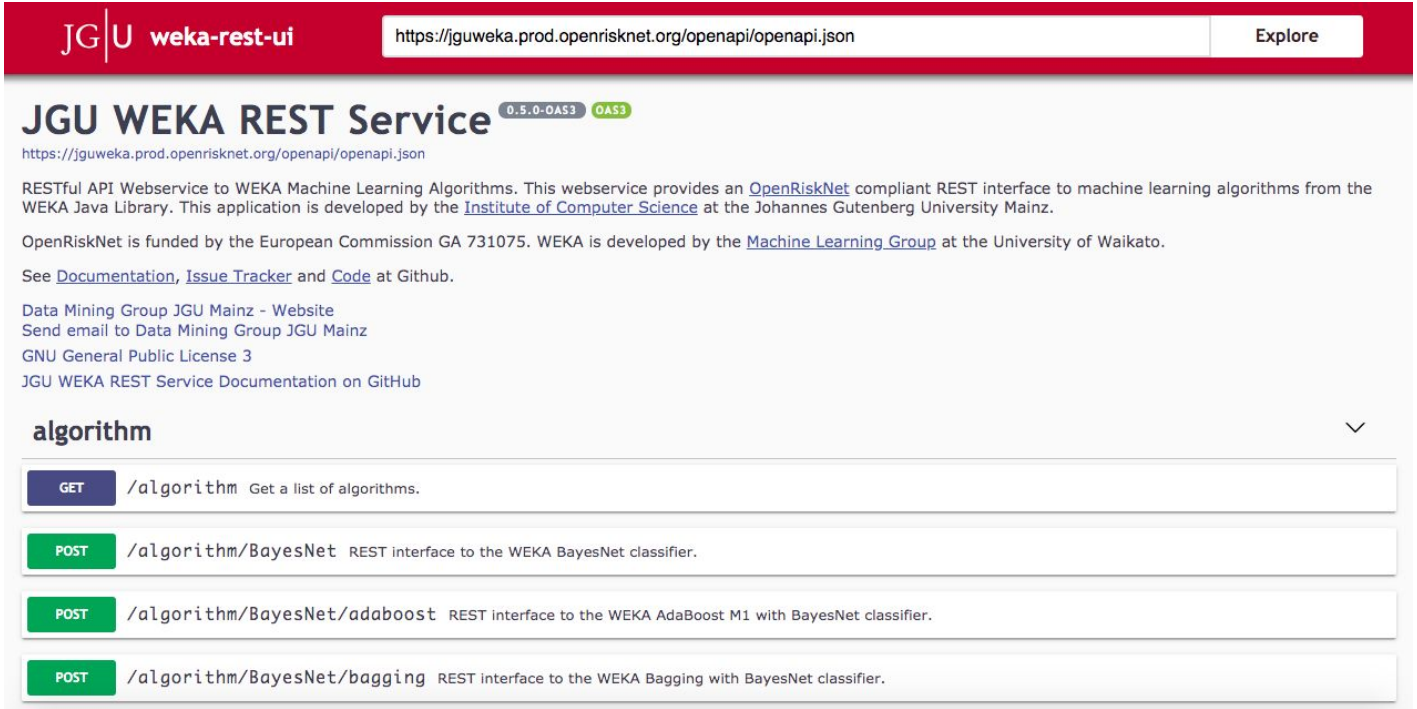
A modular framework for predictive toxicology.





Similar to the read across procedure in toxicological risk assessment, lazar creates local QSAR models for each compound to be predicted.

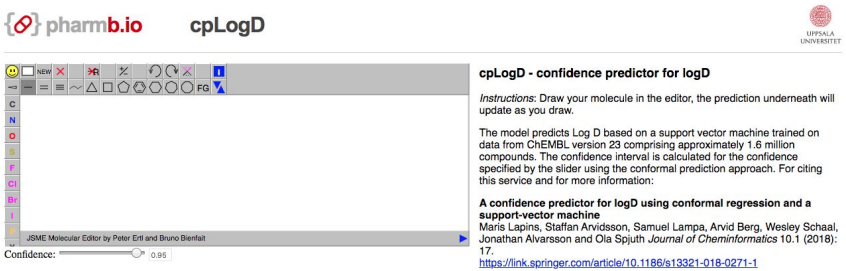
WEKA services (JGU)

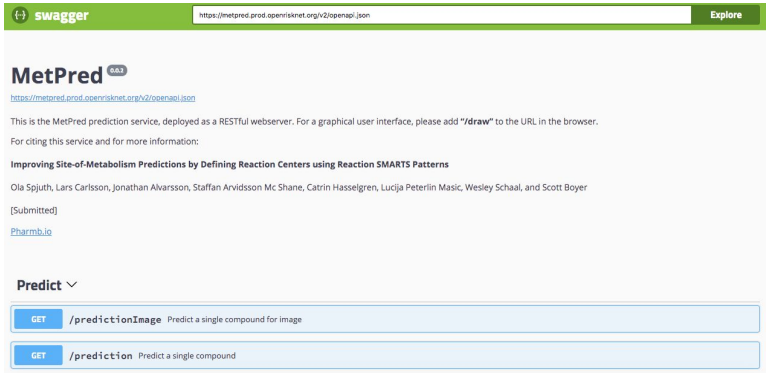


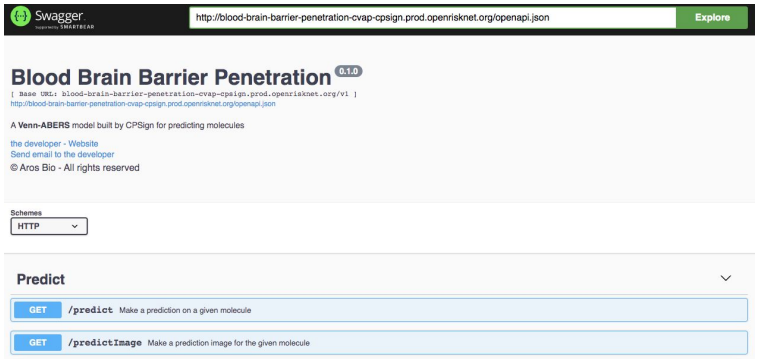
The WEKA modelling web-services by JGU provide an OpenRiskNet compliant REST interface to the machine learning algorithms from the WEKA Java Library.

CPlogD, metpred and LTKB predictions (UU)

- CPlogd (UU): (UI)
- Metpred (UU) (UI)
- LTKB (UU): Classification for LTKB data (No vs most, No vs less, No less vs most)
- Blood-brain-barrier-penetration (UU): (API) Venn-ABERS model Classification model

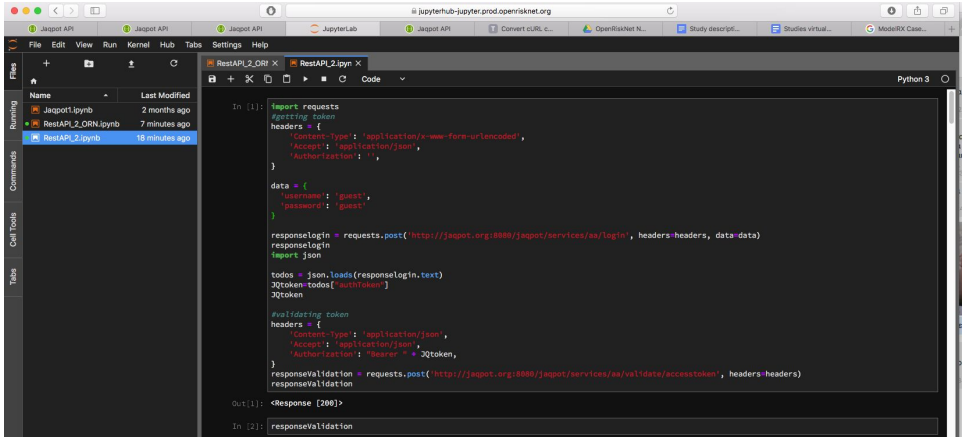




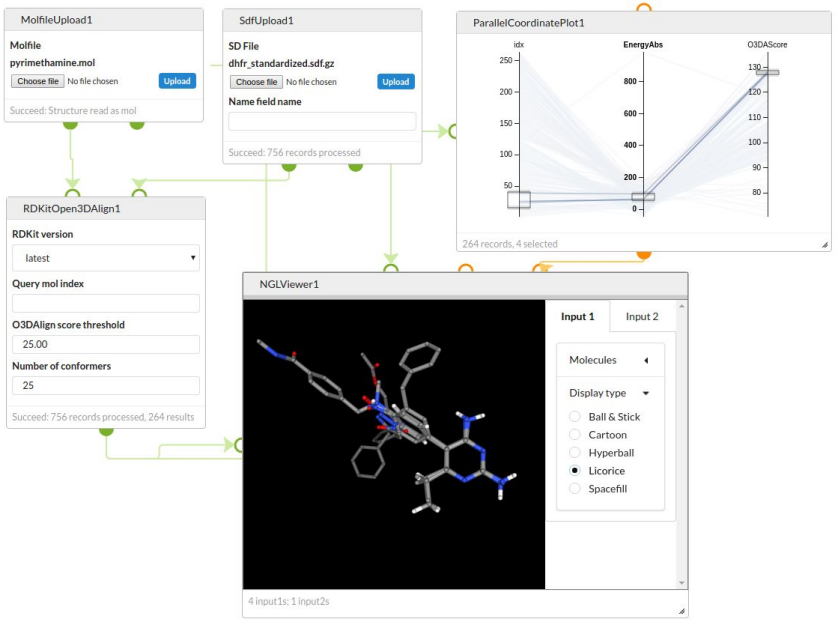


Jupyter & Squonk (IM)

Jupyter Notebooks (UI)
Squonk Computational Notebook (UI)



Jupyter notebooks infrastructure



Squonk Computational notebook

Consensus modelling (EwC)