Jaqpot

A computational cloud platform supporting the design of safe and sustainable chemicals and materials

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http://chemeng.ntua.gr/labs/control_lab/

Need addressed

The successful introduction of innovative advanced materials and chemicals (AMCs) requires an **optimal balance of safety, sustainability, functionality and cost-efficiency,** especially in a safe-and-Sustainable-by-Design (SSbD) Framework.

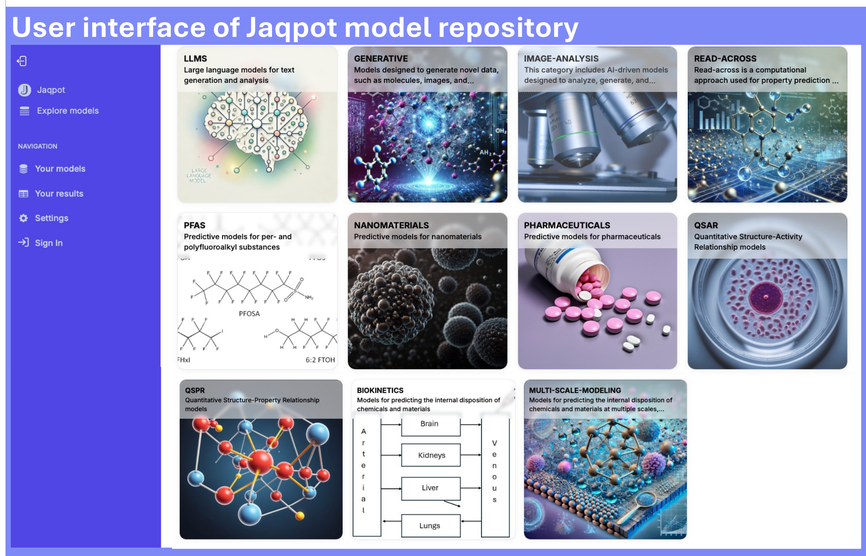
Computational approaches aim at implement the "by-Design" approach by formulating and solving **optimization problems that identify combinations of properties** across these four categories, thereby enabling **targeted materials innovation**.

This challenge is addressed by Jaqpot, **an open-source platform designed to facilitate the development, deployment, and management of machine learning (ML) models and other computational models,** specifically **tailored for chemicals and materials modelling applications** (https://app.jaqpot.org/).

Create and share models

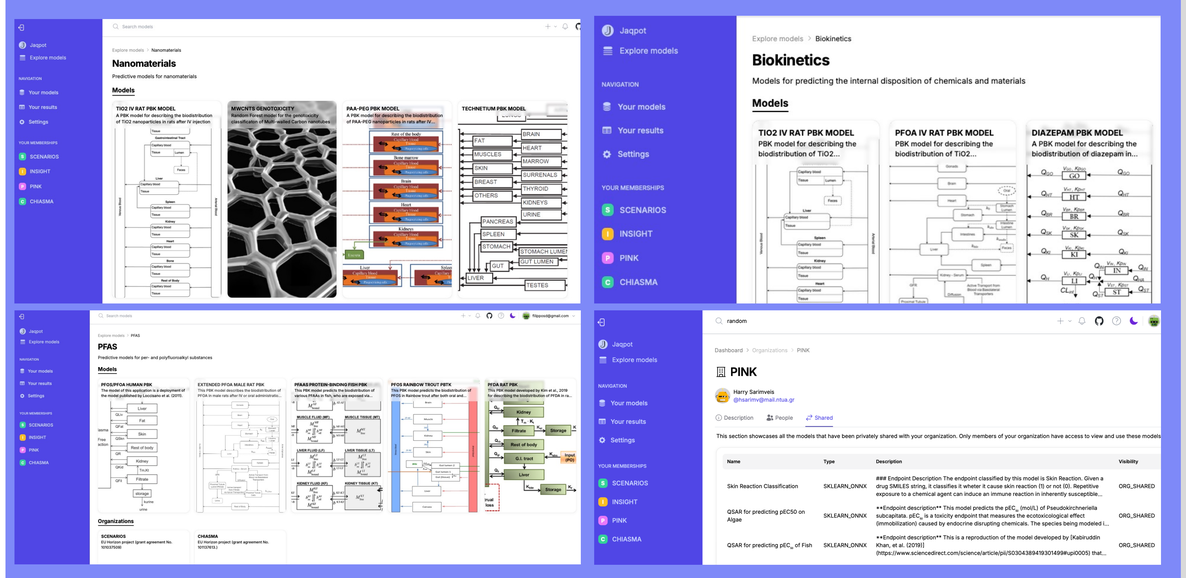
Use models

User interface of Jaqpot model repository

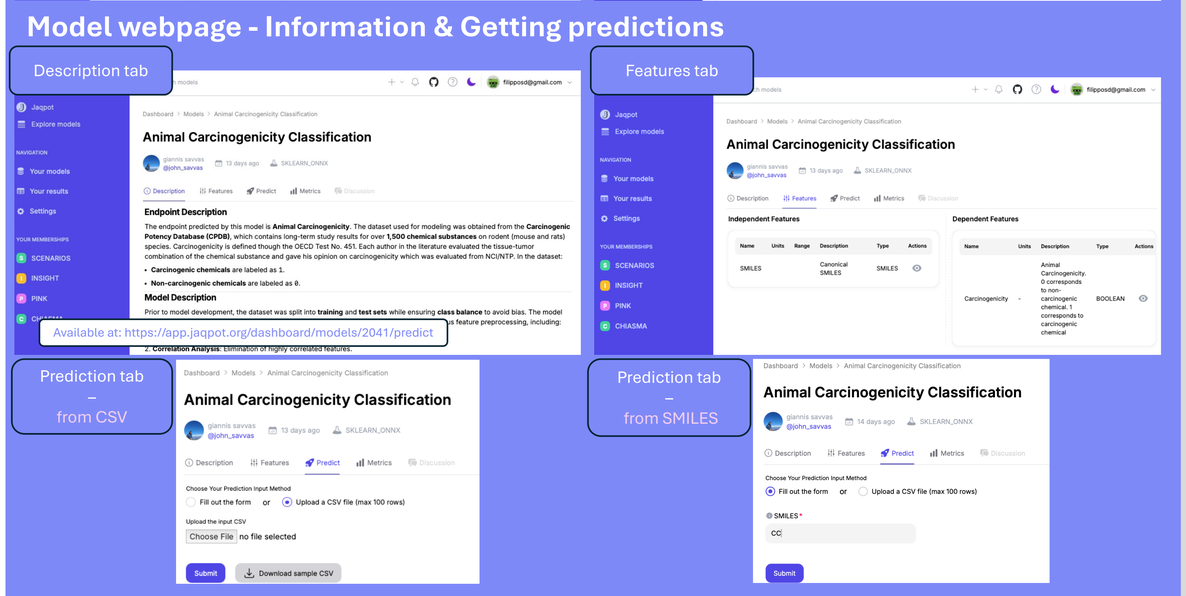


Access a repository of ready specialized models

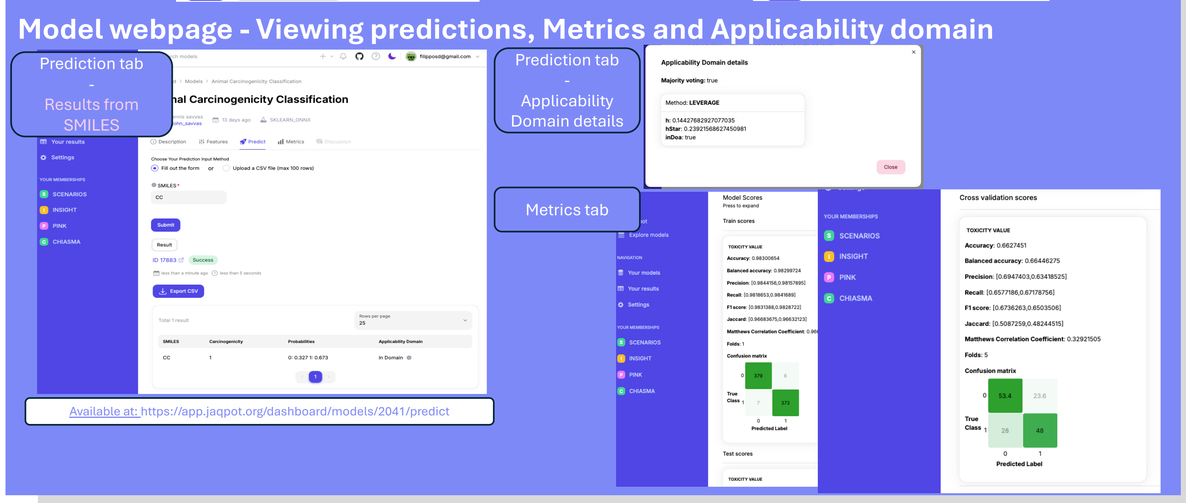
Models organised by category – Publicly available or shared within organisations



Model webpage - Information & Getting predictions

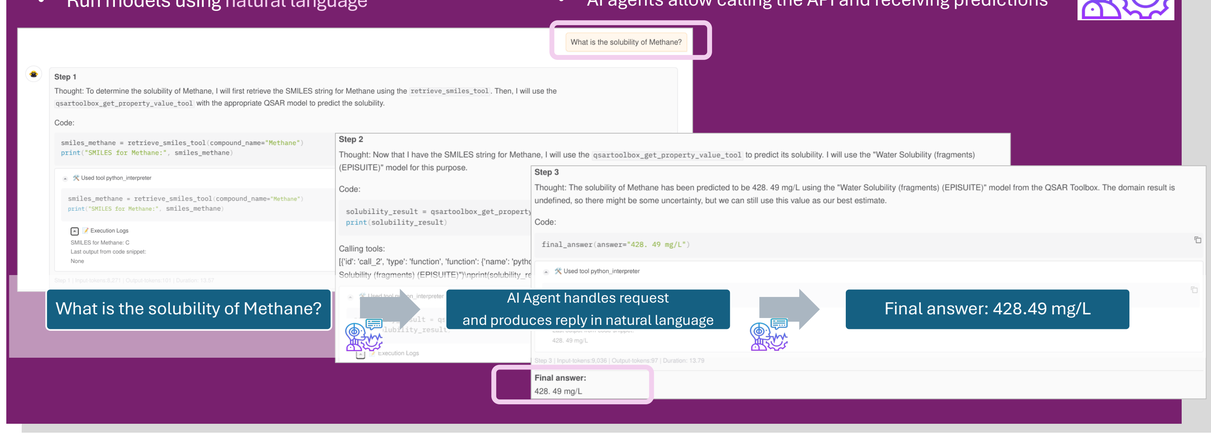


Model webpage - Viewing predictions, Metrics and Applicability domain



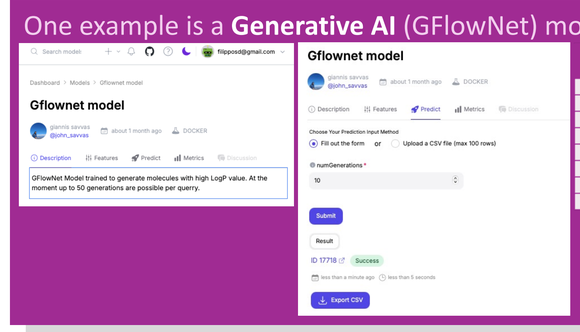
AI agents for SSbD - Conversational support for Chemical &Materials design

- Run models using natural language
- AI agents allow calling the API and receiving predictions



Harness Generative AI to generate new structures with desired characteristics

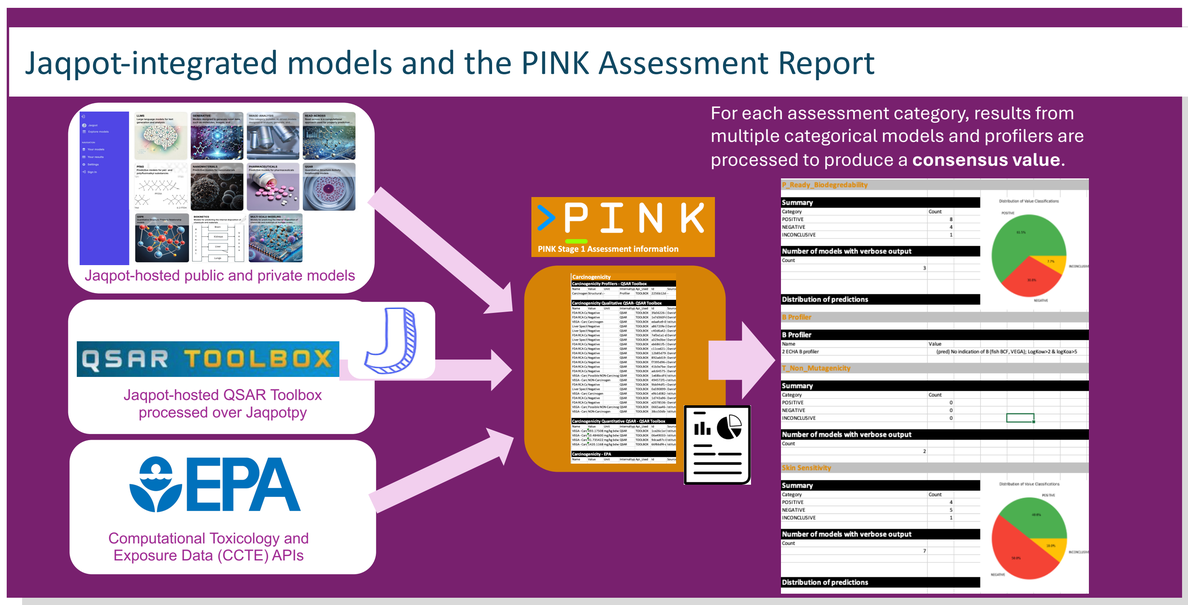
One example is a **Generative AI** (GFlowNet) model that generates molecules with high LogP values



SMILES	Prediction	QSAR Toolbox predictions
0c1cc(C2=CC(C3C=COCC3)CCC2)cc(-c2ccc3ccccc3c2)c1	8,277	9,657
CC(C)(C)C1C(C2=CCCCC2)CCCC1c1ccc(-c2cccs2)c1	9,521	10,776
c1ccc(-c2ccnc(-c3ccc(C4CCC(c5ccccc5)CC4)cc3)c2)cc1	8,299	8,784
c1cc(C2CC2)c(-c2ccc3ccccc3c2)c(C2COCC2C2CCCO2)c1	6,107	7,303
C1CCC(C2CC(C3CCC(C4CCCC4)CC3)CC(C3CCOC3)C2)CC1	9,373	11,195
CCc1ccc(C2OCCC2C2CCC(c3ccccc3)CC2)s1	6,581	7,751
c1n[nH]c(C2CCCCC2)c1C1CCCCC1C1CCCCC1N1CCNICC1	5,097	6,886
N=Cc1c(-c2cncnc2C2CCCC2)ccnc1-c1ccccc1	2,868	4,966

logP predictions for a set of generated structures were produced by QSAR TB over Jaqpot. GenAI predicted values show good agreement with QSAR TB calculated values.

Jaqpot-integrated models and the PINK Assessment Report



Conclusion

- **ML model repository** with specialized cheminformatics features
- **Python integration** through **Jaqpotpy** library
- **Support for various ML frameworks** (Scikit-learn, PyTorch Geometric)
- **Domain of Applicability** (DOA) features **specific to chemicals**
- Supports **FAIR** data and model practices
- Advanced **preprocessing and featurization** capabilities
- **API** access for programmatic integration

Available now

Acknowledgements

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SCAN ME

Try Jaqpot at https://app.jaqpot.org