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# AI-based predictive modeling for the development of SSbD chemicals & IAMs

QSAR LAB

## ABOUT QSAR Lab

We digitally design chemicals and materials to ensure their safety and compliance with the principles of sustainable development.

**35** **Experts** with

**200** **Sci. publications**

**20** **Years of experience** used in

**16** **EU-funded Projects** for total amount of

**59** **Millions EUR** in cooperation with

**190** **Partners** including: OECD, Harvard, Health Canada, UoB, Karolinska Institute, Sorbonne University, BASF etc.


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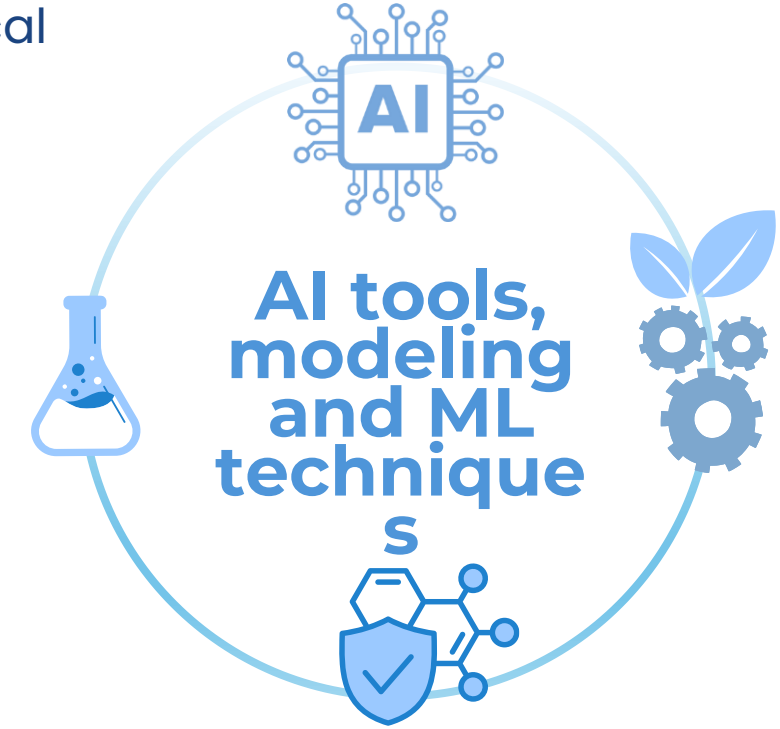
# AI-based predictive modeling for the development of SSbD chemicals & IAMs

search for alternative **IAMs** (e.g. that fulfill the technical functions of PFAS)

predict the toxicity, biodegradability, and properties of the **IAMs**, ensuring their **ssbd**

optimize the design processes with the **most efficient method**




identify the best **IAMs components** at the earliest possible stage

predict missing data points, automate data collection, processing, and analysis (e.g. to improve **LCA models)**

**virtual screening** for alternatives to hazardous materials

optimize the **recycling processes** by predicting the outcomes of different recycling techniques and identifying the best conditions

Project Idea

**Expertise offered:**

- Innovative advanced (nano)materials design
- Digital (eco)toxicology supported with ML and AI
- AI-driven algorithms and IT tools development
- Advanced data analysis
- Chemical hazard assessment
- In silico support for evaluating PFAS alternatives
- Cutting-edge predictive models
- Custom QSAR model development
- Safe and Sustainable by Design approach

| | |
|---|---|
| Organization name, town and country | QSAR Lab<br>Gdańsk, Poland |
| Addressed topic(s) | Expertise relevant to multiple topics |

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# The main calls that interest us

QSAR LAB

HORIZON-CL4-2025-05-**MATERIALS-42**
IAMs, AI/ML-driven optimization and design, SSbD

HORIZON-CL4-2025-05-**MATERIALS-43**
IAMs, AI/ML-driven optimization and design, SSbD

HORIZON-CL4-2025-05-**MATERIALS-51**
Safe alternatives for PFAS, AI/ML, SSbD

HORIZON-CL4-INDUSTRY-2025-01-**DIGITAL-61**
IAM, prediction of materials property, AI for materials science, alternatives to hazardous materials, ML for materials science

HORIZON-CL4-INDUSTRY-2025-01-**MATERIALS-61**
AI/ML-driven optimization of the recycling process; data-driven models

HORIZON-CL4-INDUSTRY-2025-01-**MATERIALS-52**
AI/ML tools to predict missing data; integration of LCA with QSAR models; AI tools to data collection, SSbD

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# Contact details

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