

Short Introduction to OpenRiskNet

The OpenRiskNet Consortium

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



Before we start

- We would like to record the meeting and make it available on the webpage (not the questions and answers)
- We would appreciate if you would tell us a little bit about you → <https://goo.gl/forms/aNo7ws7l0ysEyjuC3>
- Or even better: Fill in the complete requirement survey → <https://goo.gl/forms/xeV0xA5PTLMqpl2s1>

Agenda

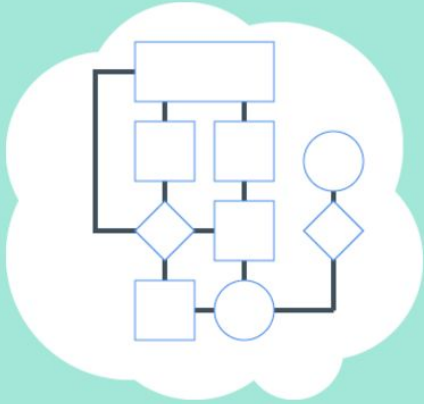
1. Introduction to OpenRiskNet project (Thomas Exner) (15 min)
2. Introduction to OpenRiskNet e-infrastructure (Tim Dudgeon) (15 min)
3. Case studies (Thomas Exner) (15 min)
4. Demonstration on OpenRiskNet services (30 min):
 - a. Jaqpot - GUI, API, workflow (Philip Doganis)
 - b. QSAR with CPSign (Conformal Prediction, CPlogD, metpred, Modeling Web, Predictive Target Profiles) (Jonathan Alvarsson)
 - c. Jupyter notebook: TG-GATEs, BridgeDb, WikiPathways (Thomas Exner)
 - d. Squonk Computational Notebook (Tim Dudgeon)
5. Associate partner programme - implementation challenge (15 min)
6. Questions and answers

OpenRiskNet - Risk Assessment E-Infrastructure

OpenRiskNet is a 3 year project with the main objective to develop an open e-Infrastructure providing **resources and services to a variety of communities requiring risk assessment, including chemicals, cosmetic ingredients, therapeutic agents and nanomaterials**. OpenRiskNet will work with a network of partners, organized within an **Associated Partners Programme**.

Large databases and highly sophisticated methods, algorithms and tools are available for different tasks such as hazard prediction, toxicokinetics, and in vitro – in vivo extrapolations to support this transition. However, since these services are developed independently and provided by different groups world-wide, there is **no standardized way to access the data or run modelling workflows**. To overcome the fragmentation of data and tools, OpenRiskNet will provide **open e-Infrastructure resources and services** supporting different scientific communities.

How?



Easily accessible
Standardised
Harmonised
Scalable
Robust
Infrastructure

For whom?



Researchers
Risk assessors
Regulators
Informed public

To what end?



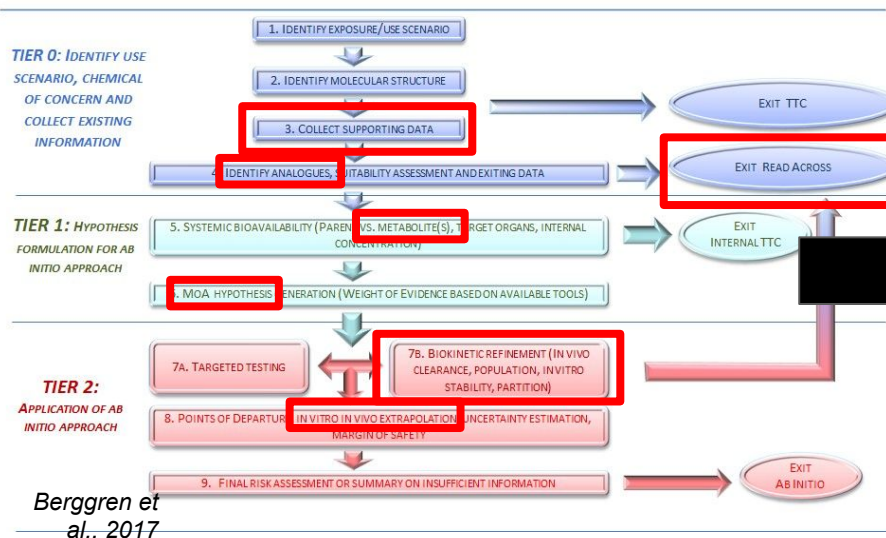
Improve industrial risk assessments
Prototyping new services and apps
Enabled access to integrated resources
Complete and qualified system
Support inovative product development

Develop + Deploy Integrated, Secure, and Sustainable e-Infrastructure

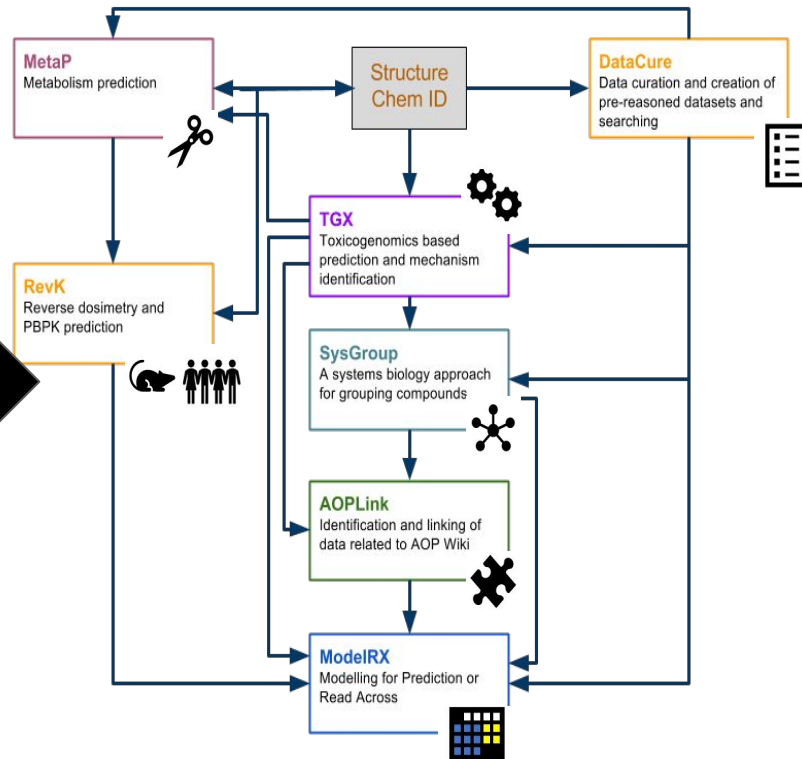
Main components of OpenRiskNet

1. **Case-study-driven development** - examples of tools to be integrated are selected based on the case study needs
2. Information on case studies in the areas of **chemical and nanomaterial risk assessment** can be found at <https://openrisknet.org/development/case-studies/>
3. Solutions for all areas by **integrating existing tools** from consortium and associated partners
4. **Integrated approach** combining experimental data (*in vivo, in vitro, in chemico*) with analysis, modelling and simulation tools to workflows for exposure, hazard and risk assessment
5. Early testing by **all stakeholder groups**

Case studies based on risk assessment framework



Berggren et al., 2017



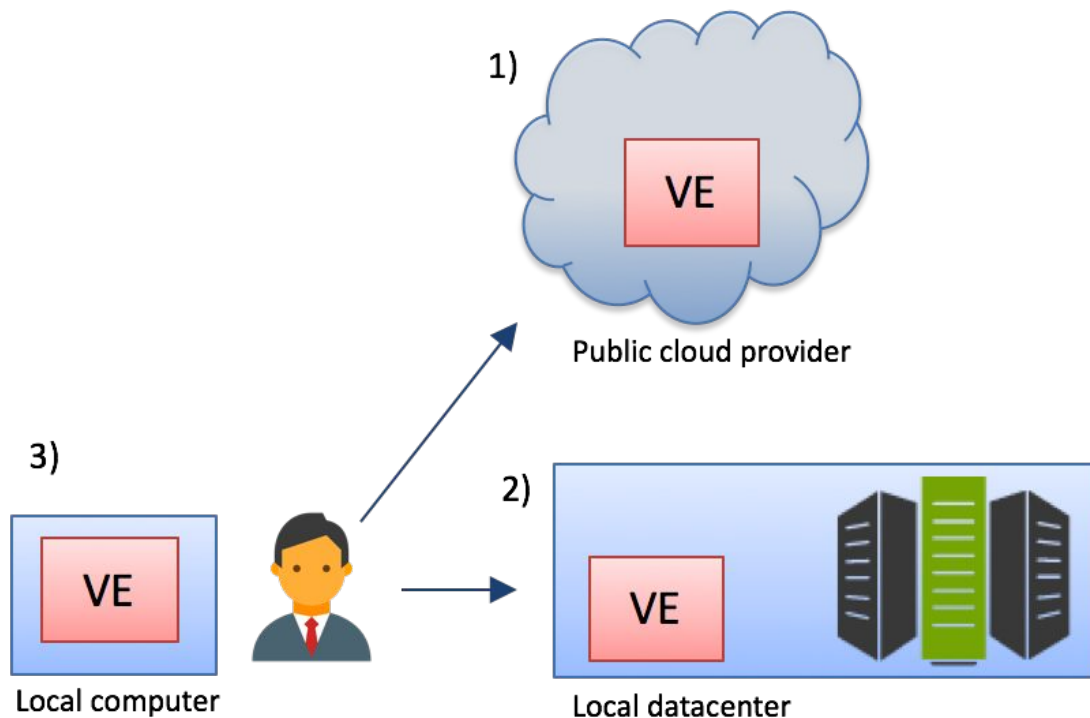
Main components of OpenRiskNet - technology

1. **REST services** providing data and processing/analysis/modelling tools (provided by OpenRiskNet and associated partners)
2. Concept to **harmonize APIs** in an bottom-up approach is available at <https://openrisknet.org/development/api-concept/>
3. No strict standards but communication through **semantic interoperability layer**, which provides information on the usage of the data and software including human- and computer readable input/output annotations.
4. Microservice architecture based on **containerization and container orchestration** accompanied by a **discovery service**
5. **Virtual infrastructures**, which can be deployed on public or in-house clouds - reference environment available at <https://home.prod.openrisknet.org>

Services

Task	Services integrated	1	2	3	4	5	6	7	8
4.1	Squonk services for chemical property prediction			x		x			
	cpLogD - confidence predictor for logD		/	x	x	/			
	Modelling Web			x		x			
	CDK-Depict			x					
	Chemidconvert	x		x	x	x	x		x
	eNanoMapper - nanomaterial database	x							
	ToxRefDB	x		x					/
	ToxCast/Tox21 summary data	x		x	x				/
	Tox21 sample specific data	x							
	FDA Estrogenic Activity Database	x	/	x	x	x	x		/
4.2	Toxygates	x		x					
	diXa (via BioStudies)	/							
	Gene Expression Omnibus (GEO)	/							
	ArrayExpress	/							
4.3	BridgeDb	x		x		x		x	
	Data mining algorithms through Jaqpot	x	/	x	x	x	x	/	/
	Data mining algorithms through JGU Weka	x	/	x	x	x	x		/
	SCAIView Scientific Literature Database	/	/	x	/				x

Virtual research infrastructures



Reference VRE

Publicly accessible reference VRE:
<https://home.prod.openrisknet.org/>

OpenRiskNet e-infrastructure

Welcome to The OpenRiskNet reference site.
This page provides a temporary landing page for end users that lists the available resources. The page is (manually) updated when new resources become available.

You will need to login to access some of these sites. Instructions on how to login can be found [here](#).

OpenRiskNet and Thrid-Party Workflow Managers and Scripting Tools

- [Squonk Computational Notebook](#)
- [Jupyter Notebooks](#)

Graphical User Interface Access to OpenRiskNet Applications

- [Lazar Toxicity Predictions](#)
- [Jaqpote Modeling and Analysis Services](#)

OpenRiskNet Data Sources

API definitions or GUIs

 **lazar-rest-api**

Explore

Lazar & Nano-Lazar REST Service 1.3.0 OAS3

<https://lazar.prod.openrisknet.org/api/api.json>

REST API webservice for lazarus and nano-lazarus.

lazar (lazy structure-activity relationships) is a modular framework for predictive toxicology. With activated Authentication & Authorization, subjectid authorization token are obligatory for designated services.

[in silico toxicology gmbh - Website](#)

[Send email to in silico toxicology gmbh](#)

[GNU GENERAL PUBLIC LICENSE](#)

See also **lazar-rest** documentation on [Github](#)

Lazar Graphical User Interface

[Lazar \(GUI\)](#)

Server

api Swagger API representation in JSON

GET /api/api.json

algorithm Algorithm

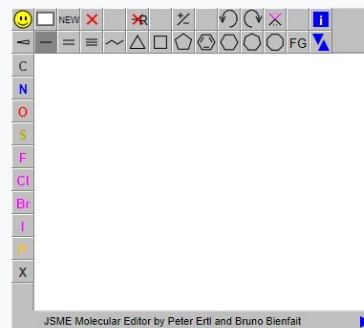


lazar toxicity predictions

Problems, bugs, ideas for improvements ? Please report at our [issue tracker](#) , check out the [FAQ](#) page or send us an email. [✉](#) [version: 1.3.1]

Please cite [DOI 10.3389/zenodo.10.3389](#) in scientific publications.

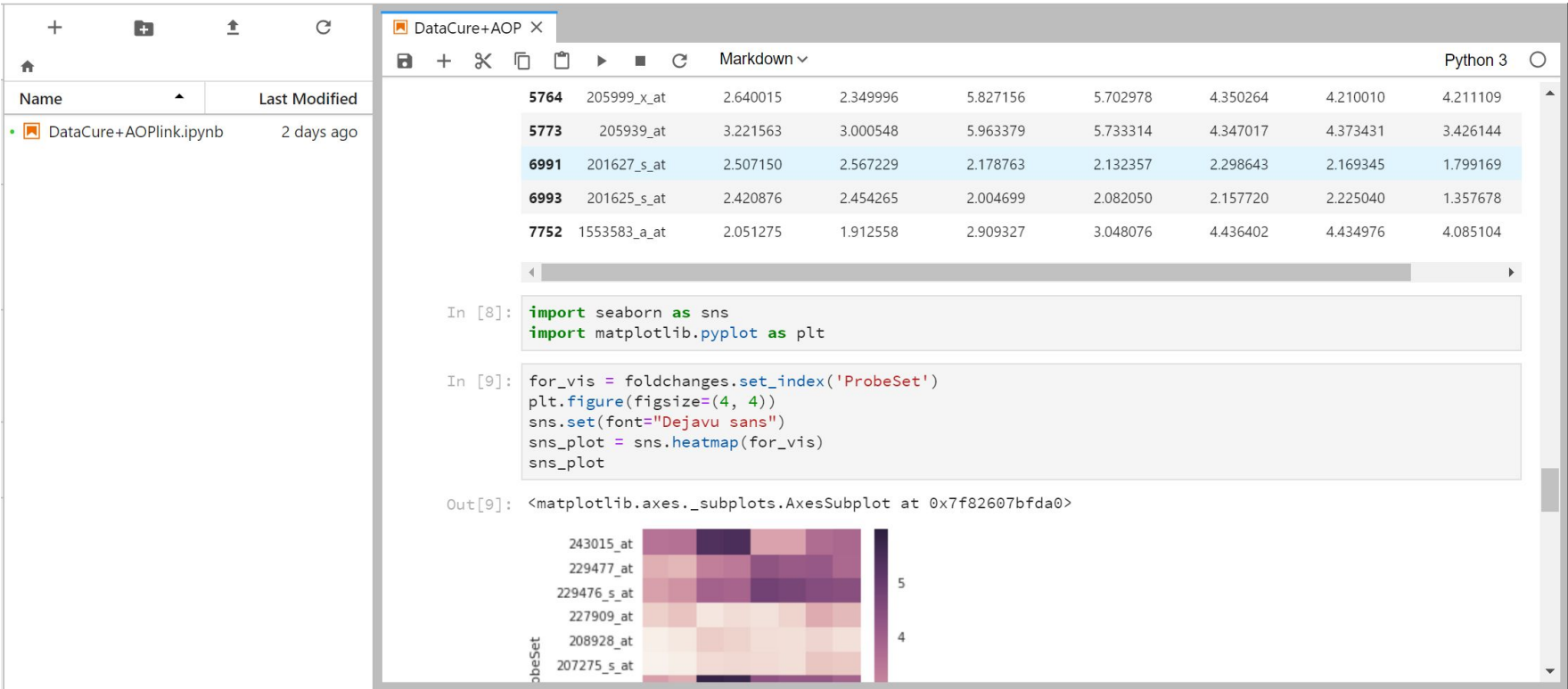
1. Draw a chemical structure



or enter the [SMILES](#) string:

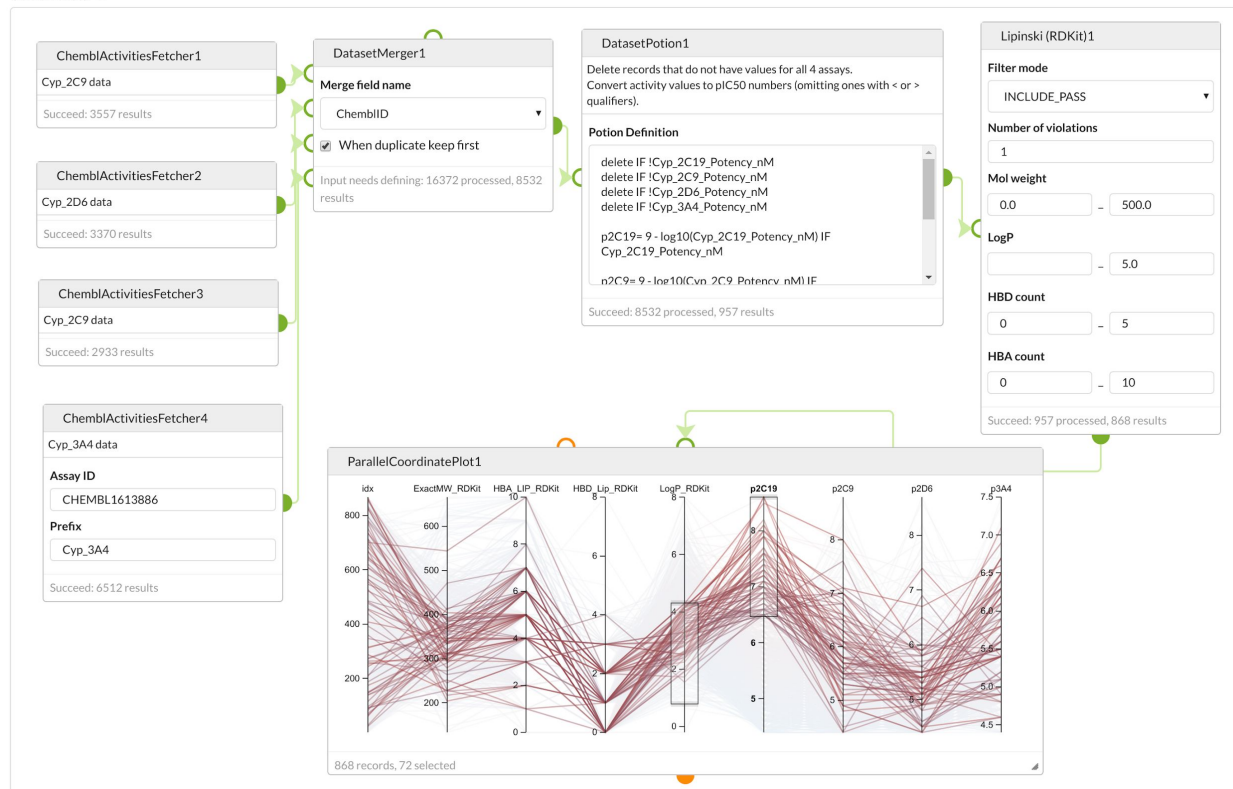
2. Select one or more endpoints

Workflow development



End user interface

CHEMBL Data - 2



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Project partners:

- P1 Douglas Connect GmbH, Switzerland (DC)
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- P4 Universiteit Maastricht, Netherlands (UM)
- P5 The University Of Birmingham, United Kingdom (UoB)
- P6 National Technical University Of Athens, Greece (NTUA)
- P7 Fraunhofer Gesellschaft Zur Foerderung Der Angewandten Forschung E.V., Germany (Fraunhofer)
- P8 Uppsala Universitet, Sweden (UU)
- P9 Medizinische Universität Innsbruck, Austria (MUI)
- P10 Informatics Matters Limited, United Kingdom (IM)
- P11 Institut National De L'environnement Et Des Risques INERIS, France (INERIS)
- P12 Vrije Universiteit Amsterdam, Netherlands (VU)