OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE

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

Webinars series

Live demonstrations on the e-infrastructure deployment and the risk assessment case studies

	Topic	Date & Time
Past events	Introduction sessions to the OpenRiskNet e-infrastructure	Webinar recordings: • Session 1 (24 Sep 2018) • Session 2 (27 Sep 2018) • Session 3 (4 Oct 2018) • Session 4 (30 Oct 2018)
	Learn how to deploy the OpenRiskNet virtual research environment	Webinar recordings (25 Feb 2019)
	Demonstration on data curation and creation of pre-reasoned datasets in the OpenRiskNet framework	Webinar recordings (18 Mar 2019)
Current event	Identification and linking of data related to AOPWiki (an OpenRiskNet case study)	Tuesday, **26 March 2019** 17:00 CET
Future events	The Adverse Outcome Pathway Database (AOP-DB)	Monday, **8 April 2019** 16:00 CET
	Semantic annotation	Monday, **13 May 2019** 16:00 CET
	Additional demo sessions on case studies	May - June 2019 (*to be announced*)

https://openrisknet.org/events/

OpenRiskNet - Risk Assessment E-Infrastructure

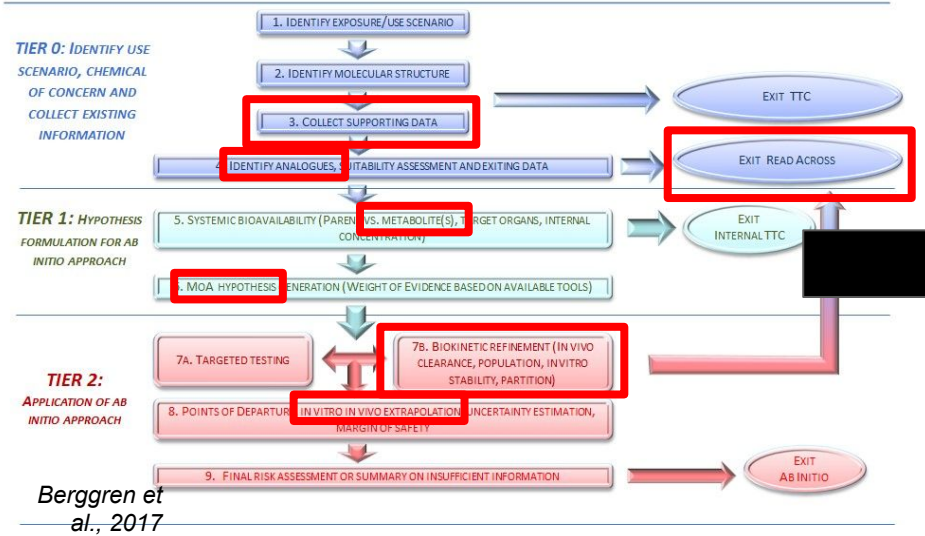
OpenRiskNet is a 3 year project with the main objective to develop an open e-Infrastructure providing **resources and services to a variety of communities requiring risk assessment, including chemicals, cosmetic ingredients, therapeutic agents and nanomaterials**. OpenRiskNet will work with a network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

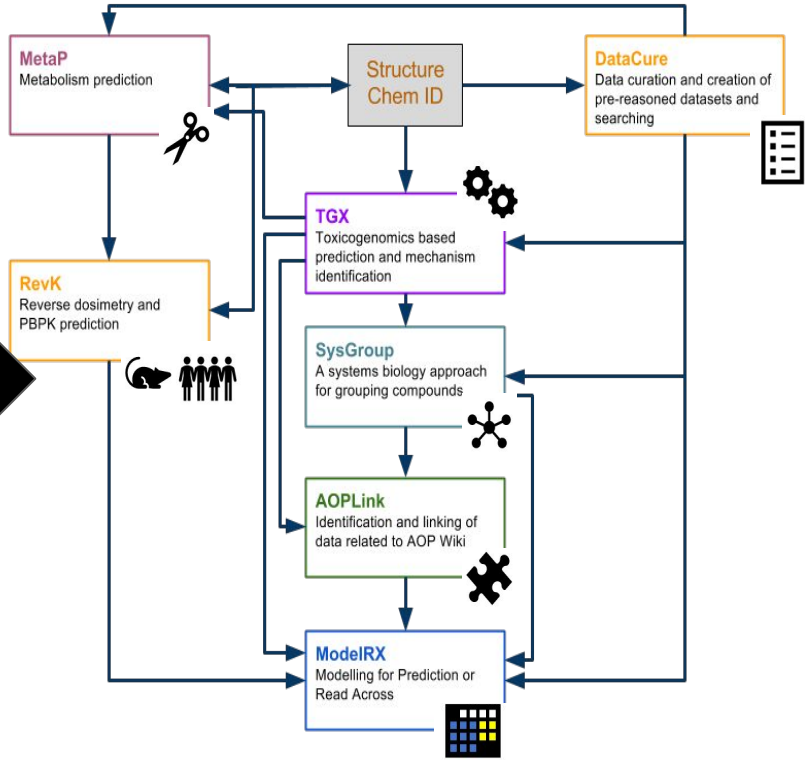
Main components of OpenRiskNet

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

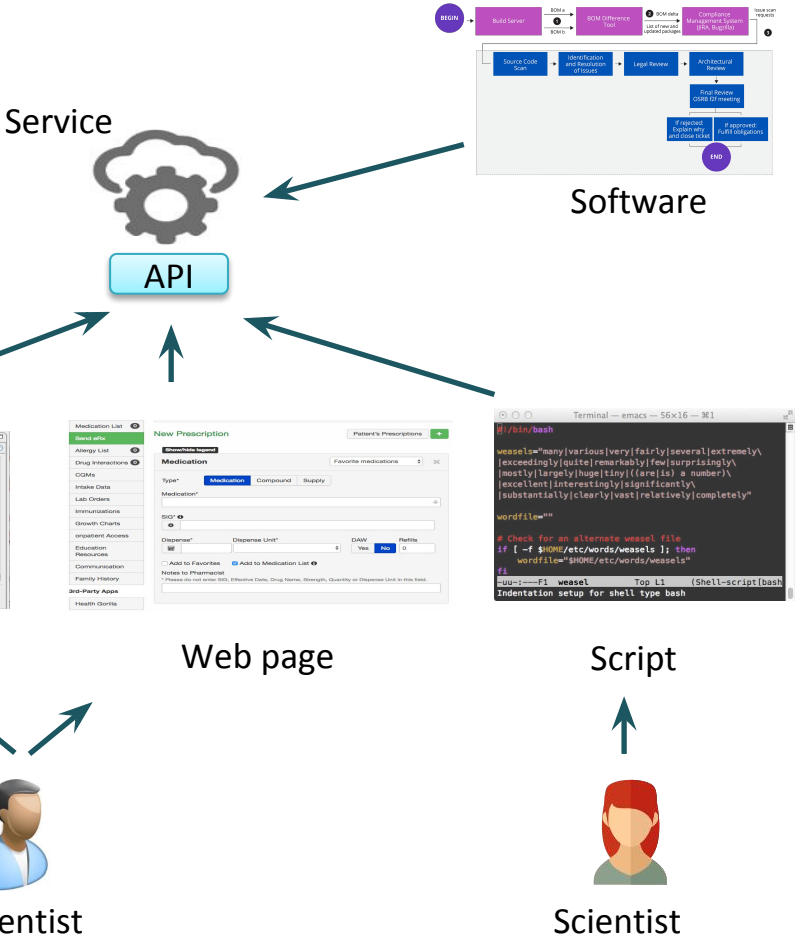


Main components of OpenRiskNet - technology

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

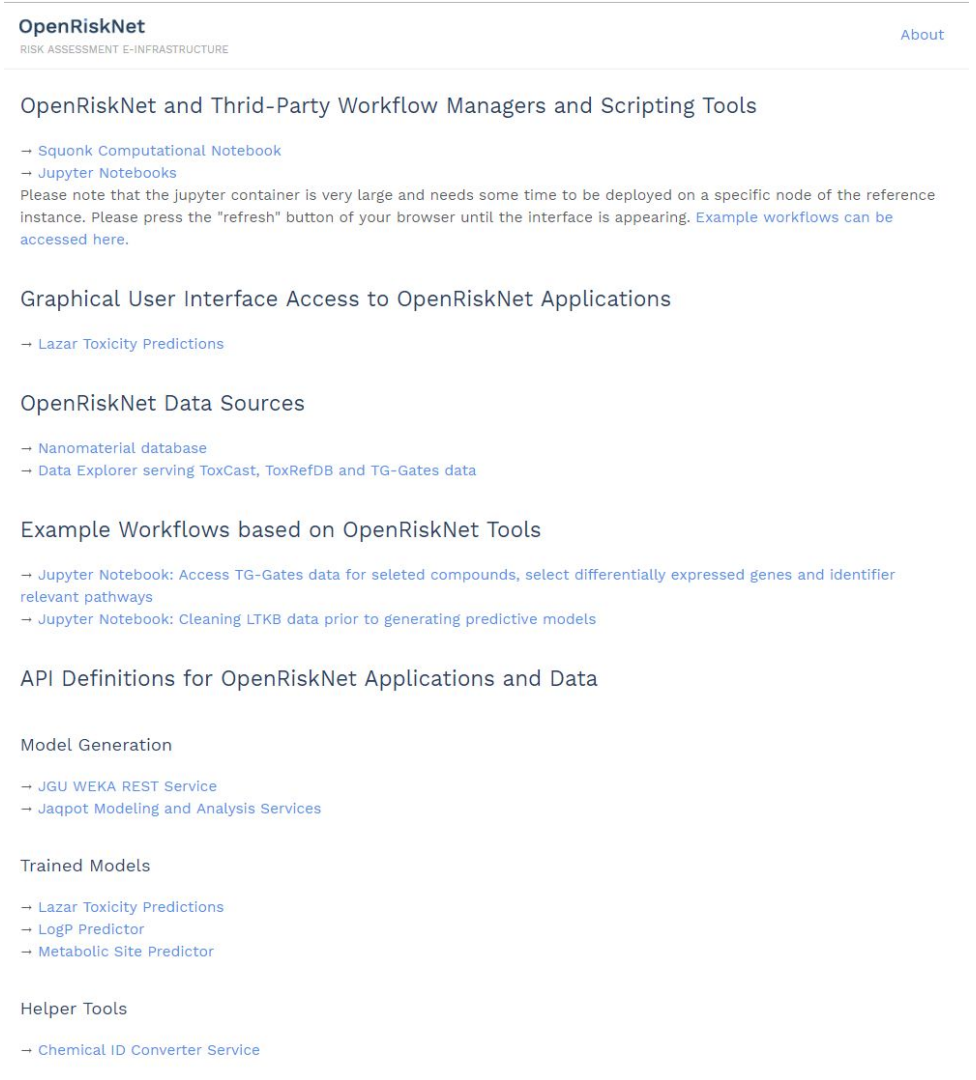
Service-oriented science

- Standardize
  - Agree on e.g. interfaces, data formats, protocols etc.
- Decompose and compartmentalize
  - Experts (scientists) provides services
  - Achieve interoperability by exposing data and tools as Web services via APIs

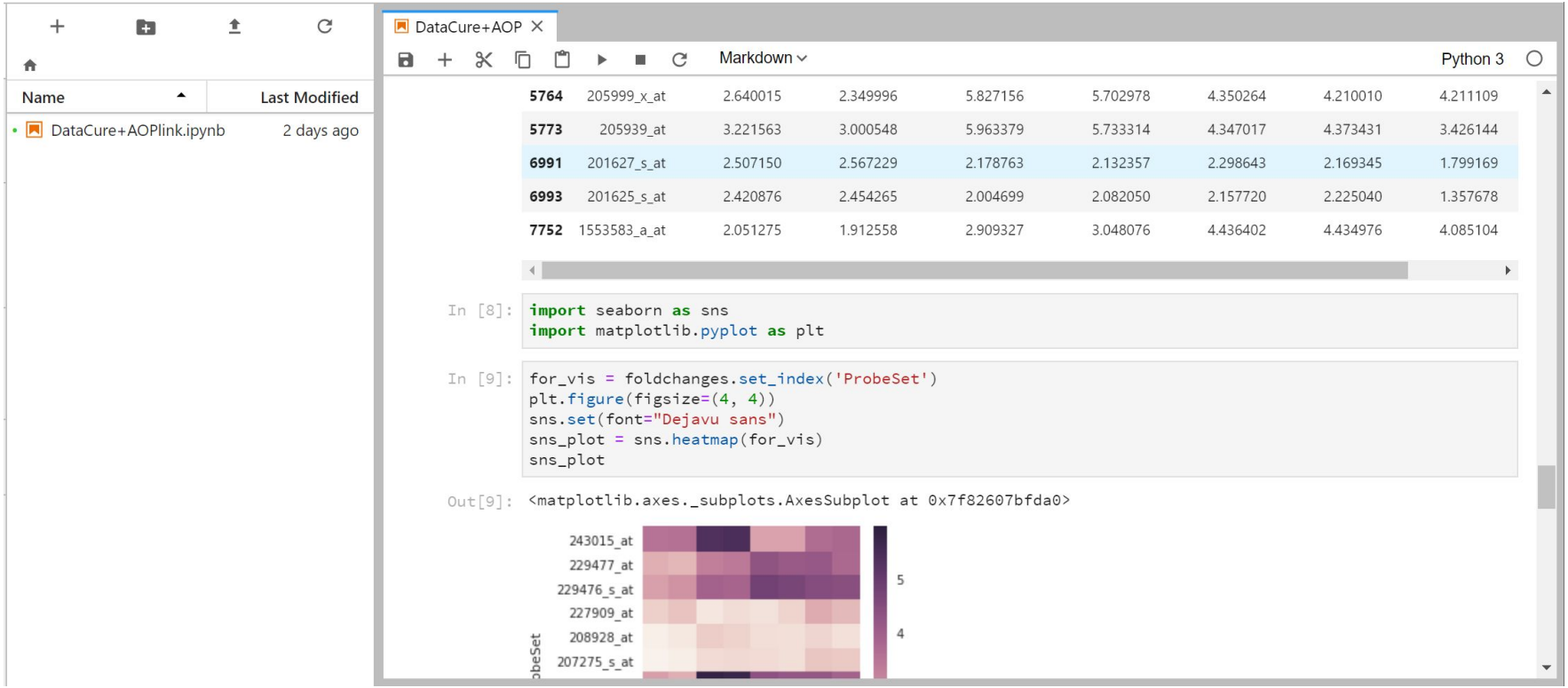


Service available

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



Workflow development



Service annotation

```
"x-orn-@context": {
  "x-orn-@id": "@id",
  "x-orn-@type": "@type",
  "@vocab": "http://openrisknet.org/schema#",
  "x-orn": "http://openrisknet.org/schema#",

  "title": "x-orn:title",
  "info": "x-orn:info",
  "paths":
    { "@id": "x-orn:paths",
      "@container": "@id"
    },
  "description": "x-orn:description",
  "unit":                    "http://pur
  "id":                      "http://eda
  "SampleID":                "http://eda
  "Substance":               "http://nci
  "Compound":                "http://nci
  "PubChemCID":              "http://sem
  "CompoundName":            "http://sem
  "InChIKey":                "http://sem
  "SMILES":                  "http://sem
  "CAS":                     "http://sem
  "Concentration":           "http://nci
  "Activity":                "http://www
}
```

Modelling

The idea was to define some key components of an OpenAPI data model for describing IC50 results that can be used by applications. It is not mandatory to use the whole model. For instance, assays are highly variable in nature so it might be more appropriate to create your own custom assay model that uses the model for an IC50 result. Alternatively the `quantity` and `quantityRange` schema object can be re-used in many other cases.

The Json Schema we defined is this (note: this is not currently syntactically correct - this will be updated soon):

```
components:
  schemas:
    quantity:
      required:
      - value
      - unit
      type: object
      description: A value with units
```

Extract compound name and concentration columns

```
substanceQuery = '''
PREFIX orn: <http://openrisknet.org/schema#>
SELECT * {
?s1 <http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C45306> ?substance .

?substance (<orn:blank>|!<orn:blank>)* ?cnameSubj .
?cnameSubj <http://semanticscience.org/resource/CHEMINF_000043> ?cnameObj .
?cnameObj <http://openrisknet.org/schema#title> ?cnameColumnheader .

?substance (<orn:blank>|!<orn:blank>)* ?concentrationSubj .
?concentrationSubj <http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C41185> ?concentrationObj .
?concentrationObj <http://openrisknet.org/schema#title> ?concentrationColumnheader
}
'''
sparql.setQuery(substanceQuery)
sparql.setReturnFormat(JSON)
sparql_result = sparql.query().convert()
SingleService = [ result for result in sparql_result if result['ServiceName'] == ORNservice]
SingleService
```

End user interface

More

Try it out

Feel free to test out one or multiple of the available services. The list of available services is constantly updated.

→ Have a look at our reference environment or
→ Learn how to set up your own VRE

Tutorials and feedback

→ Meet us – Meet us in person at one of these events.

→ Webinars – Sign up for webinars introducing the infrastructure.

→ Requirements survey – Help us optimize the infrastructure according to your needs by filling in this short survey.

→ Help desk – Report issues, give feedback and browse our knowledge base.

Acknowledgements

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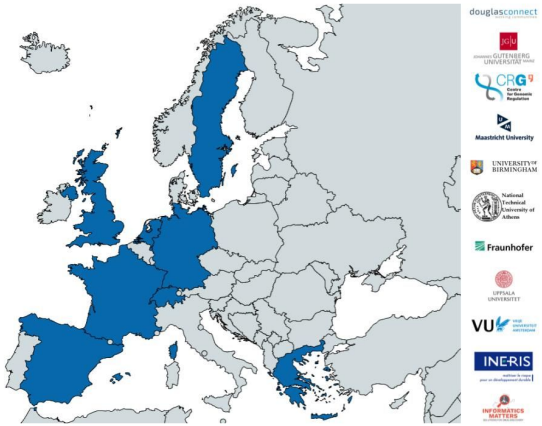
Project partners:



P1 Douglas Connect GmbH, Switzerland (DC)
P2 Johannes Gutenberg-Universität Mainz, Germany (JGU)
P3 Fundacio Centre De Regulacio Genomica, Spain (CRG)
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)
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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)