### OpenRiskNet

**RISK ASSESSMENT E-INFRASTRUCTURE** 

# Implementation Challenge and Associated Partner Programme

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



# Become involved

#### Try it out

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

- $\rightarrow$  Have a look at our reference environment or
- $\rightarrow$  Learn how to set up your own VRE

#### **Tutorials and feedback**

- $\rightarrow$  Meet us Meet us in person at one of these events.
- $\rightarrow$  <u>Webinars</u> Sign up for webinars introducing the infrastructure.
- $\rightarrow$  Requirements survey Help us optimize the infrastructure according to your needs by filling in this short survey.
- $\rightarrow$  Help desk Report issues, give feedback and browse our knowledge base.



#### Meet us f2f

#### Upcoming conferences and events

#### Meet us in person at one of these events.

Conference/Event	Partners attending
EUSAAT 23-26 Sep 2018 / Linz, Austria	Douglas Connect (DC) - <i>poster</i>
UK QSAR 26 Sep 2018 / Oxford, UK	Informatics Matters Limited (IM) - <i>poster + talk</i>
French SOT 1-2 Oct 2018	
EU-ToxRisk TempO-seq 4-5 Oct 2018	Douglas Connect (DC)
WikiPathways 2018 Summit 8-10 Oct 2018 / San Francisco, CA, US	Universiteit Maastricht (UM)
OpenTox Euro 10-11 Oct 2018 / Athens, Greece	Douglas Connect (DC) National Technical University of Athens (NTUA)
US-EU Nano meeting 11-12 Oct 2018 / Washington, DC, US	Douglas Connect (DC)



#### www.openrisknet.org

#### Survey

What best describes your role? \*

Tool developer

Data manager

Infrastructure provider

Other:

What is your experience working with HTTP based APIs (REST or similar)?

What is an API?

O I use APIs occasionally

- O I use APIs on a daily basis
- O I develop APIs

What is your experience working with service containerization?

] None

OpenRiskNet is following the concept of semantic annotation of services, which can be used by the user or other services to get information on the capabilities of the tools and the input/output options (see <a href="https://openrisknet.org/development/semantic-interoperability/">https://openrisknet.org/development/semantic-interoperability/</a> for more information). Would it be possible to annotate your service following the proposed combination of OpenAPI and JSON-LD? If yes, which meta-data annotations could you provide for data points, data sets, tools or workflows (e.g. short description of capacities, input /output parameters, author, links to publications, manuals and tutorials, license information, references/links to other objects, discussions, etc.)?

Your answer

OpenRiskNet is prioritising and testing it approaches based on case studies related to specific areas of risk assessment (descriptions available at

<u>https://openrisknet.org/development/case-studies/</u>). Which case studies are relevant to your area of research? And would you be willing to support their development and execution by providing expertise on how the requirements and challenges could be met?

I am interested

I have data sources to contribute



have tools /

workflows to

contribute

# Implementation Challenge

- E-infrastructure only as good as the services it offers
- OpenRiskNet consortium cannot cover all areas completely
- Select third-party tools for prioritized integration partial financially and strongly technically supported by OpenRiskNet

 6.000 - 12.000 € (in-kind work contributions) will be provided depending on the complexity of the service to be integrated and the amount of adaptations needed



# Service integration procedure $\rightarrow$ 8 operations

- 1. Utilising the OpenRiskNet APIs to ensure that each service is accessible to our proposed interoperability layer;
- 2. Annotating the services according to the semantic interoperability layer concept using defined ontologies;
- 3. Containerising the services for easy deployment in virtual environments of OpenRiskNet instances;
- 4. Documenting the scientific and technical background;
- 5. Deploying the service into the OpenRiskNet reference environment;
- 6. Listing the service in the OpenRiskNet discovery services;
- 7. Listing in other central repositories like eInfraCentral, bio.tools and TeSS (ELIXIR);
- 8. Providing legal and ethical statements on how the service can be used.



# API Design Concept

A		1	L	K	T L	M	N	
JSON-LD Input					PUBLICATION_	VOLUME_ S	TART_	
"openapi": "3.0.1",								
"info": {								
"x-orn-serviceAnnotation"	: "0.0.1",							
"title": "Estrogenic Activ	vity Database (EADB)",							
"description": "NCTR has	developed an Estrogeni	c Activity Dat	abase (EADB) and	made it o	penly ava	ilable	. EA	DB
"version": "1.0.0",								
"x-orn-serviceHome": "htt	ps://www.fda.gov/Scien	ceResearch/Bic	oinformaticsTools/	Estrogeni	cActivity	Databa	seEA	DB
"x-orn-ref1": {					and the second design of the			
"x-orn-refAuthors":	"Jie Shen, Lei Xu, Ho	ng Fang, Ann M	1 Richard, Jeffrey	D Brav.	Richard S	Judso	n. G	lua
"x-orn-refTitle":	"EADB: An Estrogenic	Activity Datab	ase for Assessing	Potentia	l Endocri	ne Act	ivit	v"
"x-orn-reflournal":	"Toxicological Scienc	e".	G	,				5
"x-orn-refVear"	"2013"	TT 2						
"x-orn-ref\olume"	"135(2)"							
"v_opp_pofStaptPage"	"277"							
	2// , "201"							
x-orn-retEndPage	291 ,							
"x-orn-retPMID":	"23897986"							
},								
"v-opp-pof?" · \								

# Implementation challenge

#### Deadlines for the implementation challenges are:

30 September 2018 (will be extended), 31 December 2018, 30 April 2019

#### **Selection criteria**

- Complementary to the tools from within the consortium
  - $\circ$   $\;$  Less covered areas of the risk assessment framework
  - Combinable with data and tools already available or planned to be integrated (e.g. uses input provided by ORN partners)
- Relatively high TRL preferable with existing APIs.
- Adding requirements for the infrastructure, e.g.
  - High or highly varying demand of computer resources
  - Complex workflow linking different tools
  - Need to access commercial license



## Associated Partner Programme

Officially launched at the OpenTox Euro 2017 conference (November 2017) >> <a href="https://openrisknet.org/associated-partner-programme/">https://openrisknet.org/associated-partner-programme/</a>

- **Service providers** integrate their databases and software tools into the OpenRiskNet infrastructure:
  - greater visibility of their tools by being listed in the OpenRiskNet discovery service;
  - infinite additional features by combining with other tools;
  - support for emerging techniques like API development and containerization/deployment.
- **Early adopters** use the infrastructure for their predictive toxicology and risk assessment tasks:
  - easy access to a increasing number of tools using their preferred access route (web, workfl ow tools like knime, scripts) without the need of manually downloading of data and file conversion when moving from one tool to another;
  - $\circ$   $\;$  harmonized access for comparison of different approaches.
- **Technology partners** use their services and tools for the OpenRiskNet e-infrastructure development



# Associated Partner Programme

Standard Agreement 🗸

- 1. Service providers
- 2. Early adopters:
  - a. University of Oxford
  - b. Diamond Light Source Ltd

#### 3. Technology partners:

- a. Red Hat
- b. Swedish National Infrastructure for Computing Science Cloud









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#### **Project partners**:

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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)
P9 Medizinische Universitat 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)

