OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE

WP3 Training, Support, Dissemination

Iseult Lynch (UoB), Thomas Exner and Lucian Farcal (EwC)

General Assembly and Final Consortium meeting
22 October 2019, Amsterdam (The Netherlands)

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

WP3 Objectives

Dissemination efforts to raise the awareness of the new e-infrastructure and to reach general acceptance:

- **Communicate** the scientific and technical background, capabilities and input specifications
- Produce detailed **documentation** of the implementation steps performed on the best-practice examples
- Provide **training** on implementation of databases and tools (workshops and and hackathons), on how to use e-infrastructure (schools and data hackathons)
- Provide technical **support** for implementations of services
- Produce **guidelines** and **templates**
- Collect **protocols**
- Supporting the generation of **reports** for **regulatory** purpose
- Plan for maintenance of the services, data management and the overall **sustainability** of OpenRiskNet.

WP3 Tasks

ID	Title	Partners involved	Start month	End Month	Deliverables
T3.1	Documentation of Core Infrastructure and Deployment	IM, EwC, JGU, CRG, UM, UoB, NTUA, Fraunhofer, UU, VU, INERIS	7	18	D3.2
T3.2	Support Infrastructure	UU, EwC, JGU, CRG, UM, UoB, NTUA, Fraunhofer, VU, IM, INERIS	7	36	D3.3
T3.3	Training on Service Integration and Infrastructure Usage	UM, UoB, UU, EwC, JGU, CRG, NTUA, Fraunhofer, VU, IM, INERIS	13	36	D3.4; D3.5
T3.4	Guidelines and Training on Standard File Formats, Ontology Usage, Quality Control and Protocolling	UoB, UM, EwC, JGU, CRG, NTUA, Fraunhofer, UU, VU, IM, INERIS	13	36	D3.4; D3.5
T3.5	Dissemination, Exploitation, Data Management and Sustainability Plan	EwC, JGU, CRG, UM, UoB, NTUA, Fraunhofer, UU, VU, IM, INERIS	1	36	D.3.1; D.3.6

WP3 Deliverables

ID	Deliverable	Due month	Lead partner	Type	Dissemination level
D3.1	Initial version of data management plan Version 2 updated at M24 https://doi.org/10.5281/zenodo.2558117	6	EwC	ORDP: Open Research Data Pilot	Public ✓
D3.2	First documentation of the core e-infrastructure https://doi.org/10.5281/zenodo.1483397	12	IM	Report	Public ✓
D3.3	Fully functional support Infrastructure Version 2 updated at M24 https://doi.org/10.5281/zenodo.2558122	12	UU	Demonstrator	Public ✓
D3.4	Dissemination & Training Activities (Intermediate Report) https://doi.org/10.5281/zenodo.1479649	18	NTUA	Report	Public ✓
D3.5	Dissemination & Training Activities (Final Report)	36	UoB	Report	Public 👷
D3.6	Data management, maintenance and sustainability plan	36	EwC	Report	Public 👷

WP3 Milestones

ID	Milestone	Due month	Lead partner	Means of verification
MS1	Detailed plan for the dissemination and exploitation of the project results	6	EwC	Consortium agrees on dissemination plan ✓
MS4	Fully functional support infrastructure	12	UoB	Support tools publicly accessible ✓
MS6	Guidelines and templates established for data exchange formats	18	EwC	Specifications are reported on project website ✓

WP3 Performance Metrics

Title	Status M36
Number of workshops and hackathons (Successful delivery >= 2 (until M18) and >= 5 (until M36) training workshops or hackathons)	**9** workshops and hackathons have been organised or supported, **2** internal events and **7** external events.
Acceptance of support facilities	The support functions for OpenRiskNet are functional and available, consisting of a **helpdesk**, a **wiki**, and an **issue tracker**. On top the **service catalogue** and the Library support the user in finding and accessing the resources.
Positive feedback from external participants at the workshops and hackathons	External participants at the training events, hackathons and workshops showed great interest in the solutions provided by OpenRiskNet and reaffirmed the development plans.
Active participation to conferences and meetings (Successful delivery >= 5 (until M18) and >= 10 (until M36) participation in conferences)	OpenRiskNet partners participated in **>30 conferences, meetings or other events**, with presentations or posters or attending the sessions. The materials produced for these events are documented in the Library.

D3.6 Dissemination & Training Activities (Final Report)

- Draft (continuation of D3.4 at M18)
  https://docs.google.com/document/d/1hoVsOajeouH8x4HTrzUg7ynCjJhqfVgBvPZM2w5PQIY/edit

- To be aligned with PEDR

- Structure:
  - Dissemination & Training Activities
    - Events
      - Organisation of webinars
      - Organisation of workshops, trainings and hackathons
      - Participation at conferences and workshops
    - Resources and training materials (Library)
      - Tutorials
      - Peer-reviewed publications
    - Other dissemination and networking activities
      - Public communication
      - Development of project website
      - Interactions with EU e-infrastructure projects and initiatives

Task 3.1 - Documentation of Core Infrastructure and Deployment

The architecture of OpenRiskNet is based on **Kubernetes** for distributed container orchestration with some OpenShift specific add-ons:

- The Core OpenRiskNet Infrastructure Components are **Single Sign On** (**SSO**) for authentication and authorisation

- Consolidated logging and metrics are provisioned as part of the initial OpenRiskNet reference site https://home.prod.openrisknet.org/

- **Let's Encrypt** certificates were chosen for HTTPS connections to OpenRiskNet services.

- As an extension over plain **Kubernetes**, OpenRiskNet offers **Continuous Integration and Continuous Deployment (CI/CD)** functionality

- **GitHub** used as OpenRiskNet code repository

GitHub

- OpenRiskNet code repository: https://github.com/OpenRiskNet/ (for both, **developers** and **end-users**)

- OpenRiskNet Wiki https://github.com/OpenRiskNet/home/wiki (the main resource for developer documentation in the OpenRiskNet project)

Task 3.2 - Support Infrastructure

Issue Tracker: GitHub

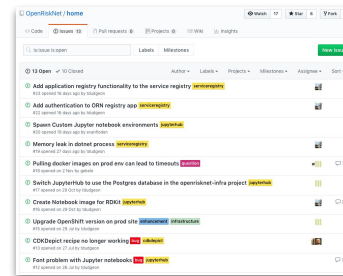**Wiki**: GitHub (key resource for supporting developers, both internal and external to the project)

Automatic testing for the virtual environments: Jenkins

Helpdesk service: https://openrisknet.freshdesk.com/
- Frequently asked questions (FAQ),
- Getting Started guide
- Form to ask questions / filing support tickets, where specified OpenRiskNet staff are responsible for handling and delegating issues

Glossary: GitHub (list of terms or abbreviations with their definition, relevant to the project)

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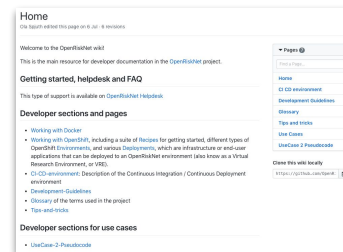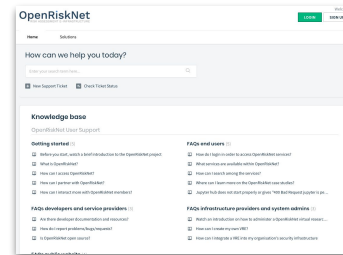**Wiki**: GitHub (key resource for supporting developers, both internal and external to the project) https://github.com/OpenRiskNet/home/wiki

Issue Tracker: GitHub https://github.com/OpenRiskNet/home/issues

Automatic testing for the virtual environments: Jenkins
https://github.com/OpenRiskNet/home/tree/master/openshift/deployments/jenkins

OpenRiskNet Services catalogue
https://openrisknet.org/e-infrastructure/services/

OpenRiskNet Library: https://openrisknet.org/library/

Support Infrastructure: end-users
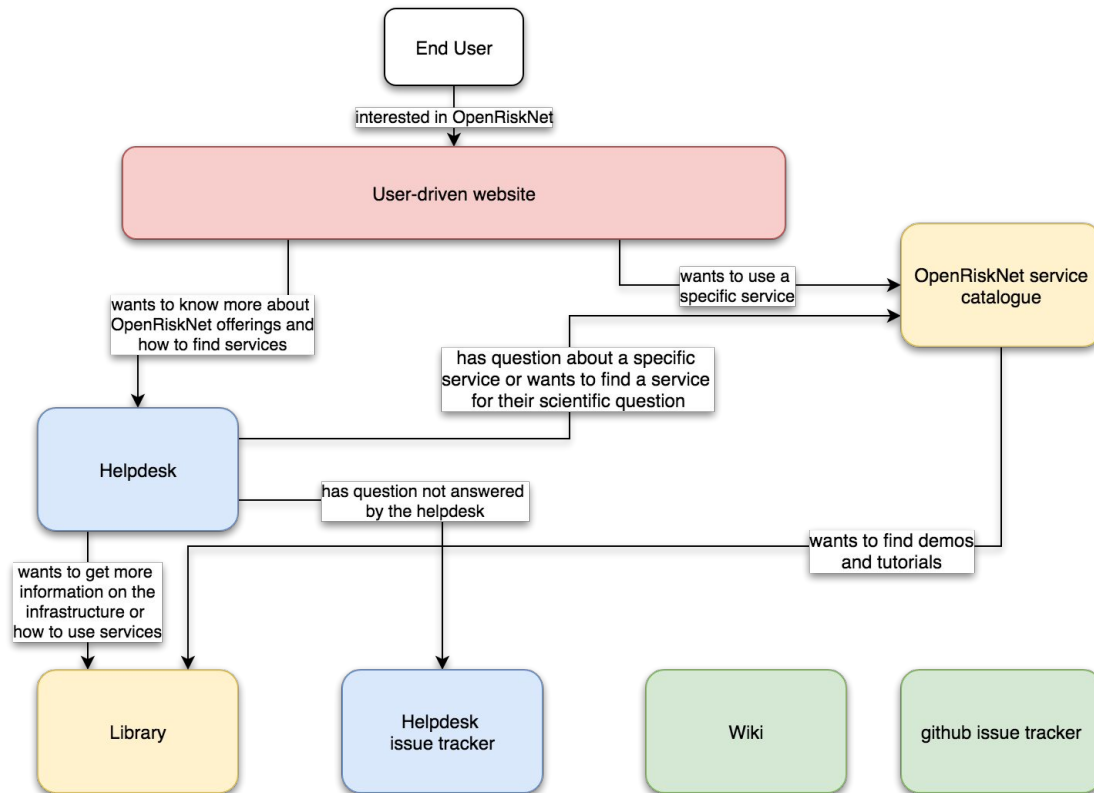
https://openrisknet.org/e-infrastructure/end-users/

End User

interested in OpenRiskNet

User-driven website

wants to use a specific service

OpenRiskNet service catalogue

wants to know more about OpenRiskNet offerings and how to find services

has question about a specific service or wants to find a service for their scientific question

Helpdesk

has question not answered by the helpdesk

wants to find demos and tutorials

wants to get more information on the infrastructure or how to use services

Library

Helpdesk issue tracker

Wiki

github issue tracker

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Support Infrastructure: service providers/developers
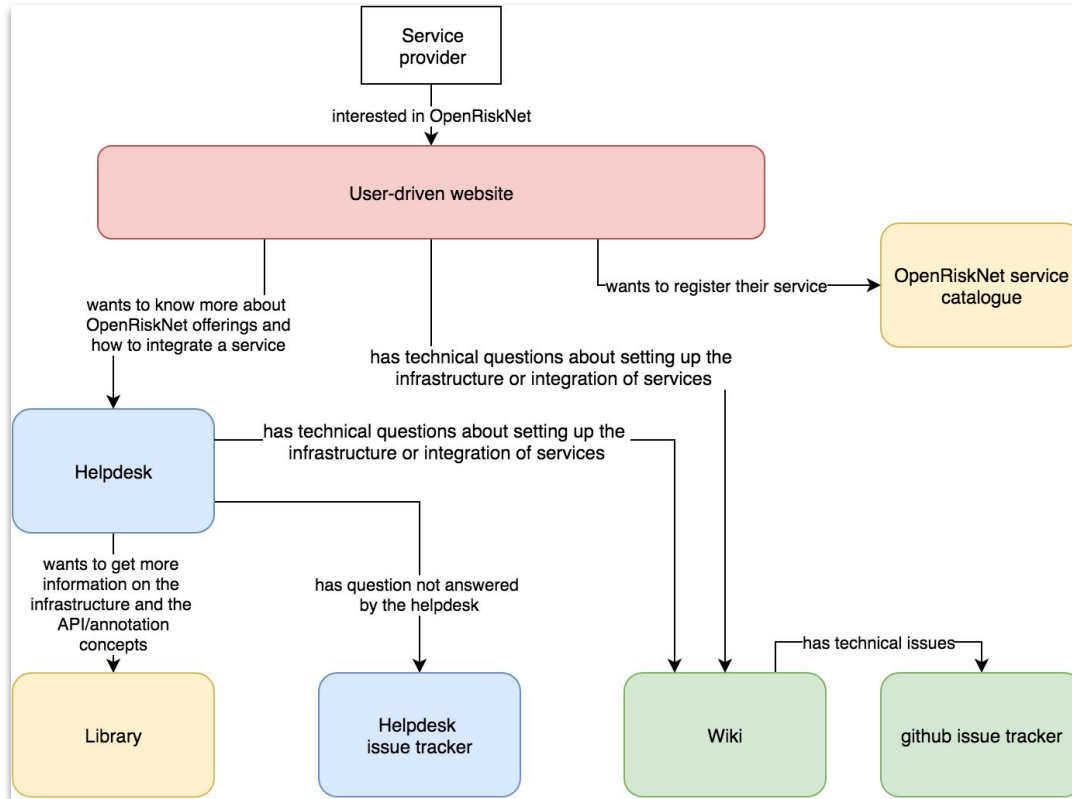
https://openrisknet.org/e-infrastructure/developers/

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Support Infrastructure: systems administrators

https://openrisknet.org/e-infrastructure/developers/

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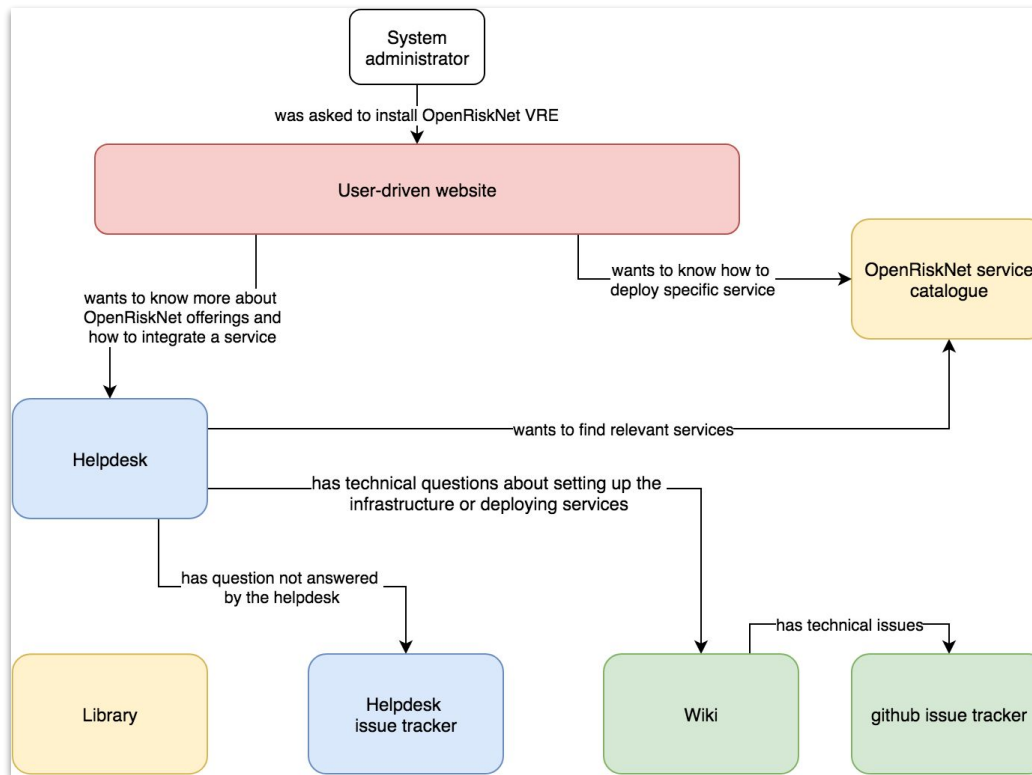
Task 3.3 - Training on Service Integration and Infrastructure Usage

- Develop **manuals, tutorials and training** material for the setup and usage of the virtual environment of e-infrastructure instances as well as integration of additional tools based on the documentation generated in Task 3.1.

- Organise **training workshops and hackathons**

  - **Implementation hackathons**: core developers and service integrators   work on the integration of specific services and provide feedback for e-infrastructure optimisation

  - **Data hackathons:** end users will bring data and case studies and work together with the service providers and core developers to execute the case studies inside the e-infrastructure

Task 3.4 - Guidelines and Training on Standard File Formats, Ontology Usage, Quality Control and Protocolling

Adoption of standards in data management, annotation, quality and reproducibility.

- Develop **guidelines for file formats, the usage of ontologies, quality control** for data and tools including measurements of uncertainty and protocolling of experimental and *in silico* procedures.

- Organise workshops to **train users outside of the consortium** and foster a general acceptance and adoption of these guidelines.

- Make the **data schemata of the OpenRiskNet services openly available** (including data/metadata file templates), which can be used as starting points for the generation of new databases but also modelling tools.

Task 3.5 - Dissemination, Exploitation, Data Management and Sustainability Plan

This task coordinated the dissemination and exploitation of the outcomes of the OpenRiskNet e-infrastructure to all stakeholders

- **Events**: https://openrisknet.org/events/
  - Conferences
  - Hackathons
  - Project meetings
  - Symposiums
  - Trainings
  - Webinars
  - Workshops
- **Resources & training**:
  https://openrisknet.org/library/
  - Peer-reviewed publications
  - Posters
  - Presentations
  - Public communications
  - Reports
  - Tutorials
  - Webinar recordings
- **News and communication**:
  https://openrisknet.org/news/
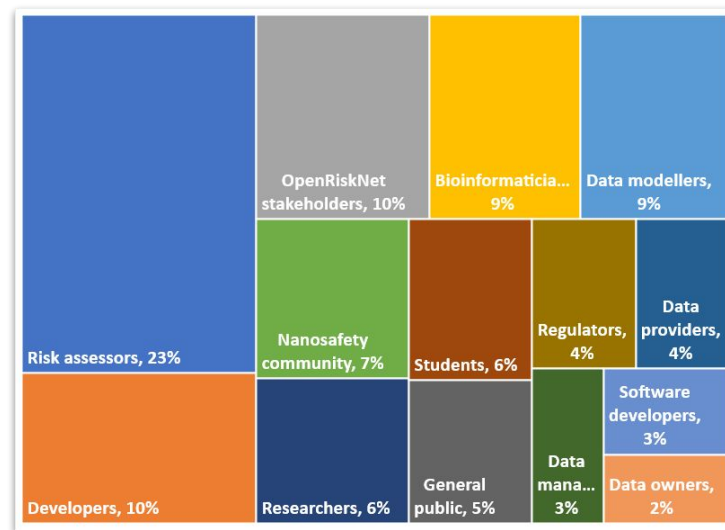
Distribution of resources to different **target audiences**

Dissemination activities
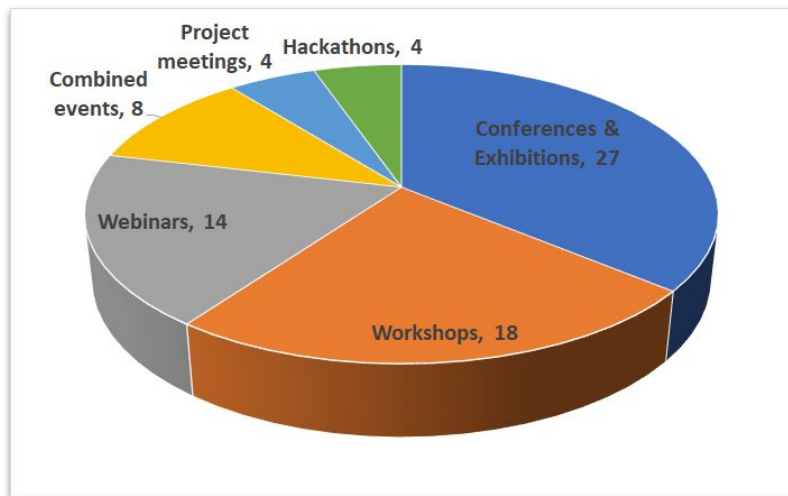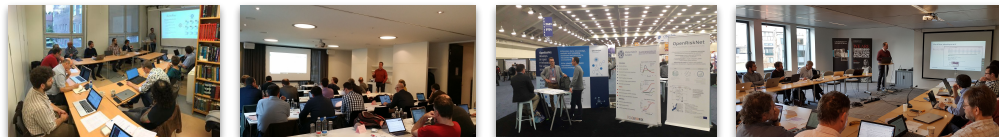
Events organised, co-organised and attended by
OpenRiskNet members
(Total: **75** by M36)
- Organiser: **22**
- Co-organiser: **22**
- Participation: **31**
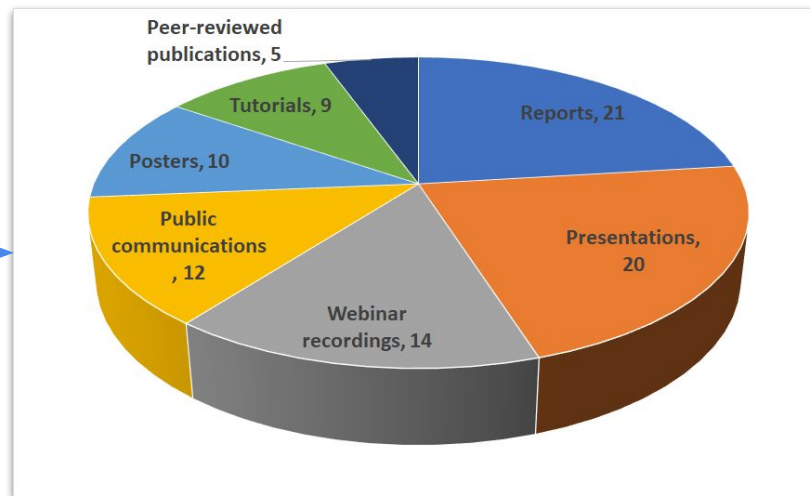
Resources & training materials available in the
OpenRiskNet library
(Total: **91** by M36)

Webinars

- OpenRiskNet webinars series included live demonstrations on the e-infrastructure deployment and the risk assessment case studies
  - Introduction to OpenRiskNet
  - Deployment
  - Demo services and case studies
  - Semantic annotations
- All sessions were recorded and the materials (slides and video) were made available in the project Library

14 Sessions

~250 Attendees

Recordings & **Slides** available

1	Introduction to OpenRiskNet project
	Edelweiss Connect, Switzerland
	11:42

2	Introduction to OpenRiskNet e-infrastructure
	Edelweiss Connect, Switzerland
	30:14

3	OpenRiskNet case studies and the implementation challenge
	Edelweiss Connect, Switzerland
	50:26

4	OpenRiskNet webinar: introduction, case studies and demo (Part 1)
	Edelweiss Connect, Switzerland
	45:23

5	OpenriskNet webinar: demonstrations on services (Part 2)
	Edelweiss Connect, Switzerland
	44:09

6	OpenRiskNet deployment
	Edelweiss Connect, Switzerland
	55:23

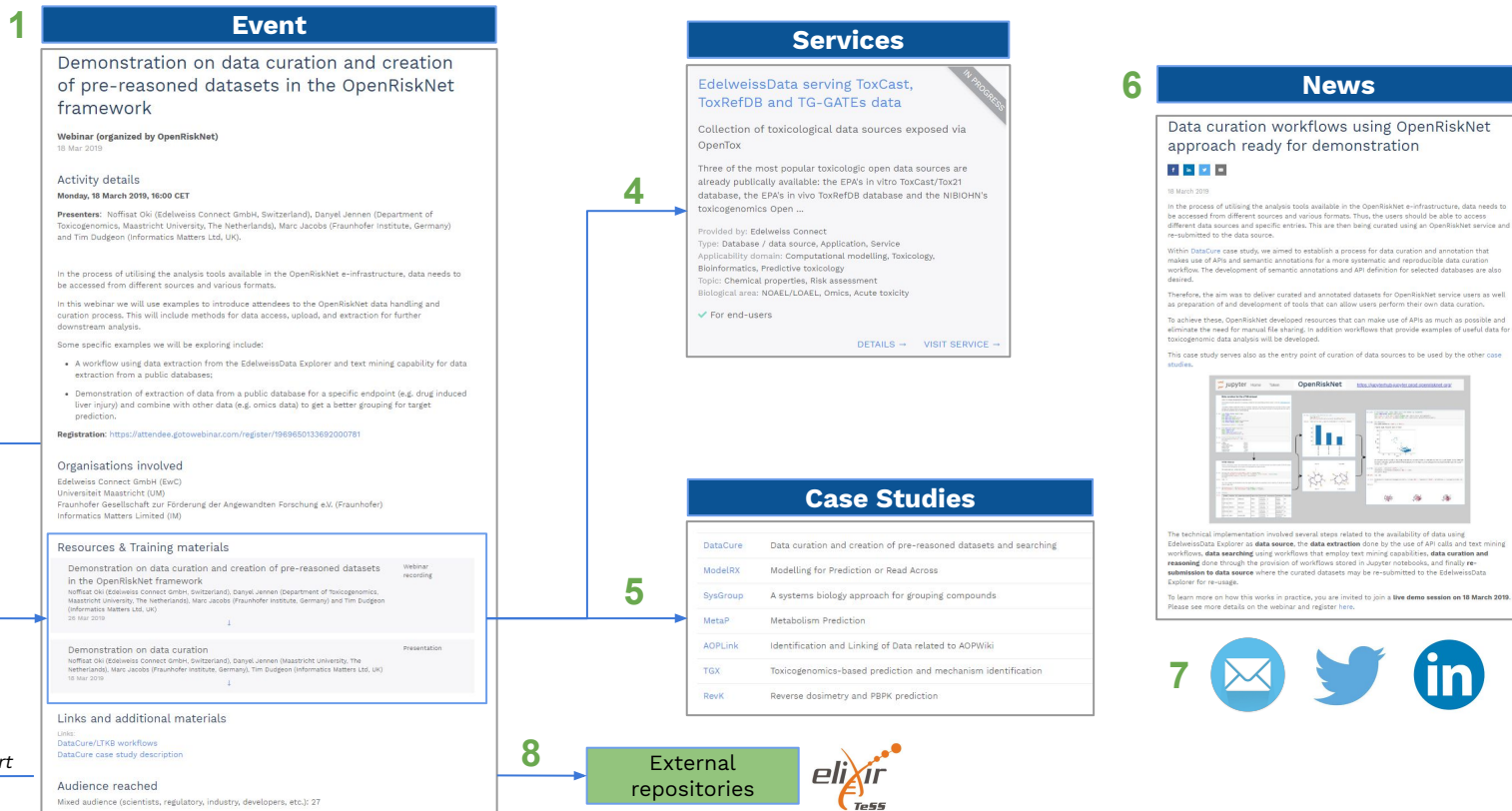| 7 | Data curation demonstration |
| | Edelweiss Connect, Switzerland |
| | 48:54 |

8	Identification and linking of data related to AOPWiki
	Edelweiss Connect, Switzerland
	52:06

9	OpenRiskNet webinar: AOP Database
	Edelweiss Connect, Switzerland
	51:42

10	OpenRiskNet webinar: Semantic annotations
	Edelweiss Connect, Switzerland
	55:23

11	OpenRiskNet Webinar: Use Nextflow for toxicogenomics-based prediction
	Edelweiss Connect, Switzerland
	54:11

12	ORN Webinar: Deploying Applications to an OpenRiskNet Virtual Environment
	Edelweiss Connect, Switzerland
	54:02

13	OpenRiskNet webinar: Approach on modelling for prediction or read across
	Edelweiss Connect, Switzerland
	56:48

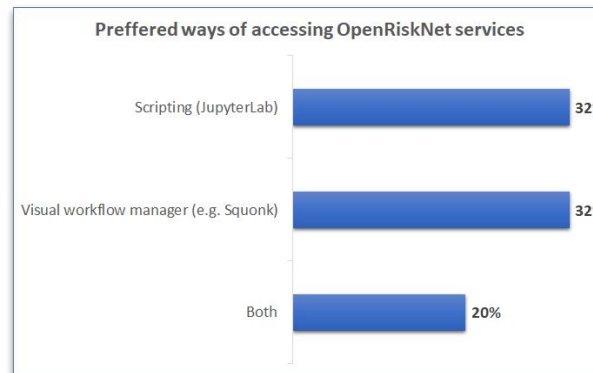| 14 | ORN Webinar: Connecting AOPs, knowledge and data with AOPLink workflows |
| | Edelweiss Connect, Switzerland |
| | 40:33 |

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Webinars

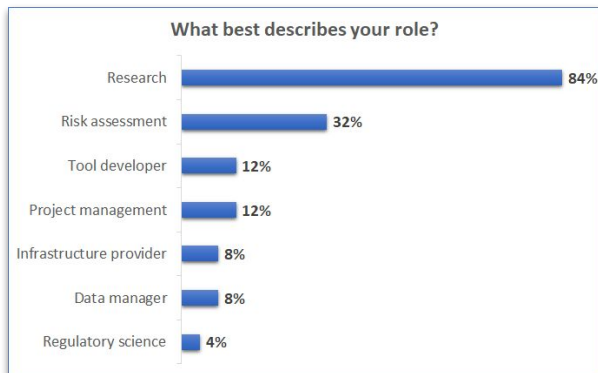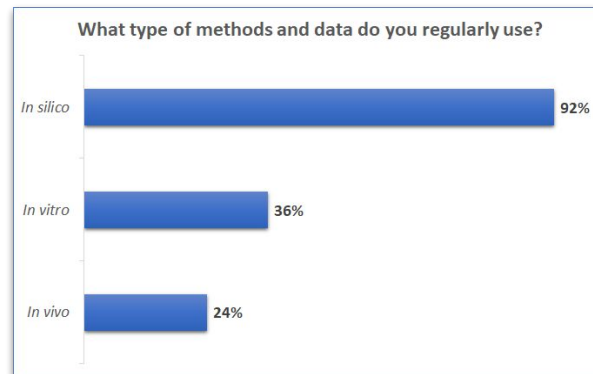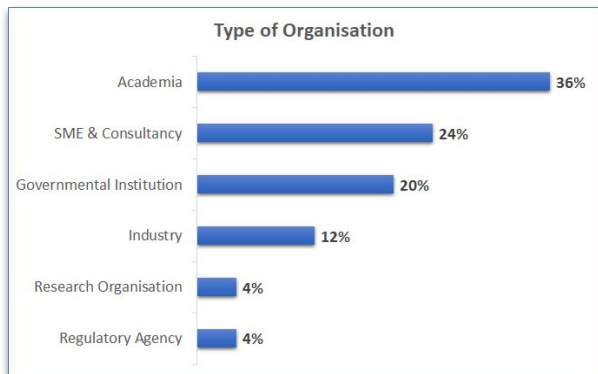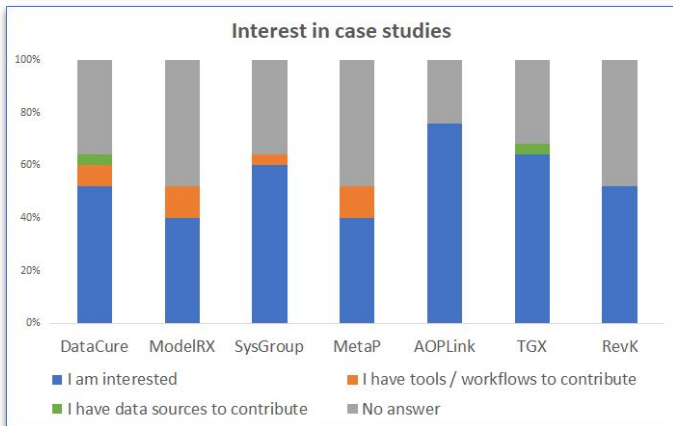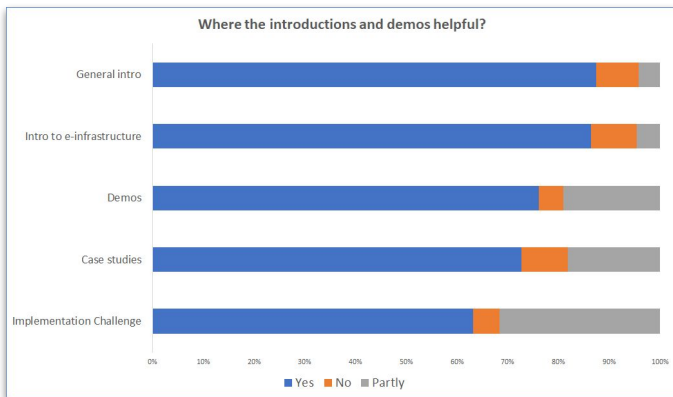| Topic	Date & Time
Introduction sessions to the OpenRiskNet e-infrastructure	Webinars description: ● Session 1 (24 Sep 2018) ● Session 2 (27 Sep 2018) ● Session 3 (4 Oct 2018) ● Session 4 (30 Oct 2018)
Learn how to deploy the OpenRiskNet virtual research environment	Webinar description (25 Feb 2019)
Demonstration on data curation and creation of pre-reasoned datasets in the OpenRiskNet framework	Webinar description (18 Mar 2019)
Identification and linking of data related to AOPWiki (an OpenRiskNet case study)	Webinar description (26 March 2019)
The Adverse Outcome Pathway Database (AOP-DB)	Webinar description (8 April 2019)
How to describe OpenRiskNet services and their functionality by semantic annotation	Webinar description (13 May 2019)
Use of Nextflow tool for toxicogenomics-based prediction and mechanism identification in OpenRiskNet e-infrastructure	Webinar description (27 May 2019)
Demonstration on OpenRiskNet approach on modelling for prediction or read across (ModelRX case study)	Webinar description (11 June 2019)
Combining neXtProt and WikiPathways strengths using SPARQL federated queries	Webinar description (12 June 2019)
Deploying Applications to an OpenRiskNet Virtual Environment	Webinar description (24 June 2019)
Connecting Adverse Outcome Pathways, knowledge and data with AOPLink workflows	Webinar description (15 July 2019)

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Example of resources generated, exploited and shared from the webinars

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Webinars follow-up survey

Type of Organisation

Academia	36%
SME & Consultancy	24%
Governmental Institution	20%
Industry	12%
Research Organisation	4%
Regulatory Agency	4%

What type of methods and data do you regularly use?

In silico	92%
In vitro	36%
In vivo	24%

What best describes your role?

Research	84%
Risk assessment	32%
Tool developer	12%
Project management	12%
Infrastructure provider	8%
Data manager	8%
Regulatory science	4%

Preffered ways of accessing OpenRiskNet services

Scripting (JupyterLab)	32%
Visual workflow manager (e.g. Squonk)	32%
Both	20%

Webinars follow-up survey

Where the introductions and demos helpful?

Categories: General intro, Intro to e-infrastructure, Demos, Case studies, Implementation Challenge
Legend: Yes, No, Partly

Interest in case studies

Categories: DataCure, ModelRX, SysGroup, MetaP, AOPLink, TGX, RevK
Legend: I am interested, I have tools / workflows to contribute, I have data sources to contribute, No answer

Suggestions from participants:

● Address more specific groups, e.g. only tool developers or only end users;

● Focused sessions, with more time focussing on case studies and demos;

● Cover different audiences (both end-users and developers);

● Follow a complete example on the e-infrastructure use;

● Build a story on how to use the integrated tools, in order to capture the attention of end users;

● The terminology may be added to explain the meaning of words in different modules;

● Allow access to the tools and support materials before the sessions;

● Explain in more detail the database access flows;

● *And many more…*

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Workshops (RP2)

Workshop sessions during OpenTox Euro Conference (October 2018 Athens, Greece)

- **Hands-on Workshop on Biokinetics Modelling**
  - Biokinetics Modelling and Simulation
  - Unknown parameter estimation using Bayesian statistics
  - Introduction to PKSim modelling platform
  - Introduction to httk R package
  - Reverse dosimetry using control theory
  - Biokinetics modelling through the Jaqpot platform

Resources & Training materials

Biokinetics Modelling: use, form, inputs and outputs of PBPK models   Tutorial
Harry Sarimveis, Aris Dokoumetzidis, Pantelis Karatzas, Philip Doganis, Periklis Tsiros, Nikolas-Marios Katritsis, Georgia Tsiliki
9 Oct 2018

→ Workshop files ↓

- **Building risk assessment workflows with OpenRiskNet**

Activity details

This workshop aims at providing the users with experience on using the OpenRiskNet infrastructure for risk assessment. Users will investigate a problem from nanosafety, studying a panel of nanoparticles (including dry powders of oxides of titanium, zinc, cerium and silicon, dry powders of silvers, suspensions of polystyrene latex beads and dry particles of carbon black, nanotubes and fullerene, as well as diesel exhaust particles). The OpenRiskNet infrastructure will be employed to generate models on the toxicity of studied nanoparticles, more specifically the Jaqpot platform for modelling, available at http://www.jaqpot.org.

Organisations involved

Edelweiss Connect GmbH (EwC)
National Technical University of Athens (NTUA)

Links and additional materials

Website:
http://www.opentox.net/events/opentox-euro-2018/s6

Links:
Jaqpot modelling platform
Workshop documents

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Workshop
Creating powerful workflows combining data and software services demonstrated on risk assessment case studies

OpenRiskNet
RISK ASSESSMENT E-INFRASTRUCTURE

23 - 24 October 2019, Amsterdam, Netherlands | https://openrisknet.org/

Final OpenRiskNet Workshop: Creating powerful workflows combining data and software services demonstrated on risk assessment case studies

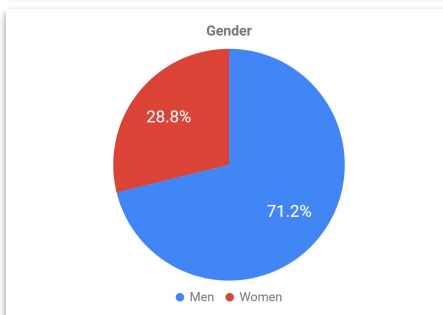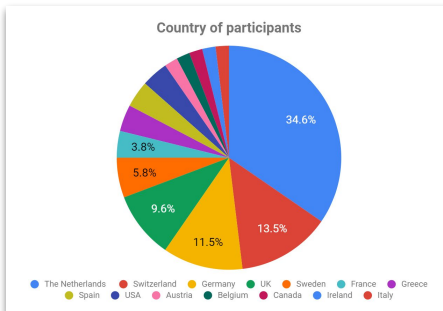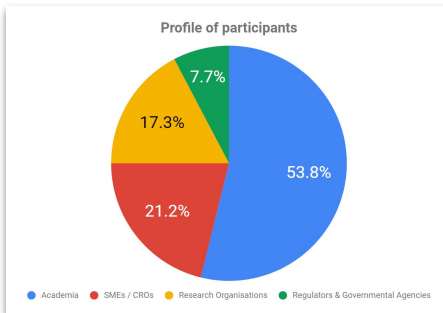**Workshop (organized by OpenRiskNet)**
23 – 24 Oct 2019 / Amsterdam, NL

- Lectures, demo & hands-on trainings
- Associated partners session
- EU infrastructures & sustainability session
- Posters session

Activity details

Venue: Vrije Universiteit, Auditorium, O|2 Human Life Sciences building, De Boelelaan 1108, 1081 HZ Amsterdam, The Netherlands (Map)

Booklet (agenda, abstract, additional information): OpenRiskNet Final Workshop

https://openrisknet.org/events/74/

Profile of participants

- Academia 53.8%
- SMEs / CROs 21.2%
- Research Organisations 17.3%
- Regulators & Governmental Agencies 7.7%

Country of participants

- The Netherlands 34.6%
- Switzerland 13.5%
- Germany 11.5%
- UK 9.6%
- Sweden 5.8%
- France 3.8%
- Greece
- Spain
- USA
- Austria
- Belgium
- Canada
- Ireland
- Italy

Gender

- Men 71.2%
- Women 28.8%

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Training & Guidelines on Standard File Formats, Ontology Usage, Quality Control and Protocolling (RP2)

1st NanoCommons Hackathon on "Ontological Annotation of Datasets"

Hackathon (co-organized by OpenRiskNet)
9 Oct 2018 / Athens, GR

Activity details

The 1st NanoCommons Hackathon on "Ontological Annotation of Datasets" was co-organised by H2020 projects NanoCommons and OpenRiskNet. The hackathon took place during the afternoon on 9 October 2018 in conjunction with the next NanoCommons Consortium Meeting (8-9 October 2018) and the OpenTox Euro Conference (8-11 October 2018) in Athens, Greece. The participants worked using their own or mock datasets and search through established ontologies (e.g. eNanoMapper Ontology) for ontological annotations. The participants also learn how to prepare electronic files (e.g. JSON) containing the raw data and the ontological metadata.

Organisations involved

Edelweiss Connect GmbH (EwC)
Universiteit Maastricht (UM)
The University Of Birmingham (UoB)
National Technical University of Athens (NTUA)

Links and additional materials

Website:
https://www.nanocommons.eu/1st-nanocommons-hackathon-ontological-annotations-of-datasets/

OpenRiskNet/NanoCommons ontology meeting

Hackathon, Workshop (co-organized by OpenRiskNet)
13 – 14 Dec 2018 / Brussels, BE

Activity details

The goal of this meeting is to get a picture of the ongoing ontology activities in the toxicology area, harmonize these efforts and the developed ontologies therein, and extend the existing toxicology ontology to support OpenRiskNet and NanoCommons tasks. Part of this will be the ontological annotation of OpenRiskNet Application Programming Interfaces (APIs) as used on their cloud. Other goals include extension of the ontology with missing terms (if any), potentially write up guidance documents, and annotation of data sets (possible via OpenRiskNet data APIs). The detailed information and agenda are available below.

Topics:

1. What ontologies are out there and can we combine them to a toxicology application ontology.

2. Data and software schema: How much ontology do we need to annotate complex services.

3. Ontology Hacking.

The complete agenda is attached below.

Registration

Organisations involved

Edelweiss Connect GmbH (EwC)
Johannes Gutenberg-Universität Mainz (JGU)
Universiteit Maastricht (UM)
The University Of Birmingham (UoB)
National Technical University of Athens (NTUA)
Fraunhofer Gesellschaft zur Förderung der Angewandten Forschung e.V. (Fraunhofer)
Uppsala Universitet (UU)
Informatics Matters Limited (IM)

How to describe OpenRiskNet services and their functionality by semantic annotation

Webinar (organized by OpenRiskNet)
13 May 2019

Webinar

Activity details

Monday, 13 May 2019, 16:00 CEST

Presenter: Thomas Exner (Edelweiss Connect GmbH, Switzerland)

Providing the data and software services within OpenRiskNet virtual environment and make the functionality available via application programming interfaces (APIs) already allows for the development of advanced workflows providing solutions to complex risk assessment tasks (demonstrated in the case studies webinars). However, identification and selection of the most appropriate service, understanding their functionality and format the input and output still need manual investigation and programming/scripting skills. To be able to automate these tasks, OpenRiskNet is exploring semantic annotation on different levels.

After a short introduction to ontologies applicable to service annotation, we will first demonstrate high-level annotation, which gives the information for the OpenRiskNet registry service to index the service and to make it findable for users and gives basic categorisation like dataset, algorithm and model. Then we will show low level annotation, which will be used for dataset and input/output harmonisation so that the user but more important other services can understand the information provided/required and how to access it. Finally, first approaches to define the middle layer providing metadata describing the service in more detail like available toxicity domains, available endpoint as well as gene/pathway/AOP associations will be shown.

Registration: https://register.gotowebinar.com/register/836537431881200140

Organisations involved

Edelweiss Connect GmbH (EwC)

Active participation in other major events (selection)

- **54th Congress of the European Societies of Toxicology (EUROTOX)**, 2 – 5 Sep 2018 / Brussels, BE
- **20th International Congress on In Vitro Toxicology (ESTIV)**, 15 – 18 Oct 2018 / Berlin, DE
- **SOT 58th Annual Meeting and ToxExpo**, 11 – 14 Mar 2019 / Baltimore, US
- **EOSC-hub Week**, 10 – 12 Apr 2019 / Prague, CZ
- **ISMB/ECCB 2019 - International Conference on Intelligent Systems for Molecular Biology & European Conference on Computational Biology**, 21 – 25 Jul 2019 / Basel, CH
- **Building EOSC through the H2020 projects current status and future directions**, 9 – 10 Sep 2019 / Brussels, BE

Complete list: https://openrisknet.org/events/

OpenRiskNet Part III: Modelling Services in Chemical/Nano-safety, Environmental Science and Pharmacokinetics
Stefan Kramer, Philip Doganis, Denis Gebele, Atif Raza, Pantelis Karatzas, Haralambos Sarimveis, Jonathan Alvarsson, Ola Spjuth, Staffan Arvidsson, Thomas Exner, Lucian Farcal, Barry Hardy
28 Aug 2019
→ doi: 10.7490/f1000research.1117419.1   ↓
Poster

OpenRiskNet Part II: Predictive Toxicology based on Adverse Outcome Pathways and Biological Pathway Analysis
Marvin Martens, Thomas Exner, Nofisat Oki, Danyel Jennen, Jumamurat Bayjanov, Chris Evelo, Tim Dudgeon, Egon Willighagen
28 Aug 2019
→ doi: 10.7490/f1000research.1117418.1   ↓
Poster

OpenRiskNet Part IV: WEKA Machine Learning Services for the Prediction of Half-Lifes of Chemicals and Nanoparticle Transport
Stefan Kramer, Denis Gebele, Atif Raza
28 Aug 2019
→ doi: 10.7490/f1000research.1117420.1   ↓
Poster

OpenRiskNet Part I: Development of an open e-infrastructure predictive toxicology and risk assessment
Thomas Exner, Lucian Farcal, Daniel Bachler, Nofisat Oki, Denis Gebele, Atif Raza, Stefan Kramer, Evan Floden, Cedric Notredam, Jordi Rambla, Danyel Jennen, Jumamurat Bayjanov, Egon Willighagen, Marvin Martens, Chris Evelo, Iseult Lynch, George Gkoutos, Philip Doganis, Pantelis Karatzas, Haralambos Sarimveis, Marc Jacobs, Ola Spjuth, Tim Dudgeon, Alan Christie, Frederic Bois, Daan Geerke, Paul Jennings, Barry Hardy
2 Aug 2019
→ doi: 10.7490/f1000research.1117259.1   ↓
Poster

Publications

Peer-reviewed publications

Population pharmacokinetic reanalysis of a Diazepam PBPK model: a comparison of Stan and GNU MCSim
Periklis Tsiros, Frederic Y. Bois, Aristides Dokoumetzidis, Georgia Tsiliki and Haralambos Sarimveis
4 Apr 2019
→ Article   ↓

Introducing WikiPathways as a data-source to support Adverse Outcome Pathways for regulatory risk assessment of chemicals and nanomaterials
Marvin Martens, Tim Verbruggen, Penny Nymark, Roland Grafström, Lyle D. Burgoon, Hristo Aladjov, Fernando Torres Andón, Chris T. Evelo, Egon L. Willighagen
4 Dec 2018
→ Article   ↓

Predicting off-target binding profiles with confidence using Conformal Prediction
Samuel Lampa, Jonathan Alvarsson, Staffan Arvidsson Mc Shane, Arvid Berg, Ernst Ahlberg, and Ola Spjuth
6 Nov 2018
→ doi: 10.3389/fphar.2018.01256   ↓

A confidence predictor for logD using conformal regression and a support-vector machine
Lapins M, Arvidsson S, Lampa S, Berg A, Schaal W, Alvarsson J, Spjuth O
3 Apr 2018
→ doi: 10.1186/s13321-018-0271-1   ↓

Semantic prioritization of novel causative genomic variants
Imane Boudellioua, Rozaimi B. Mahamad Razali, Maxat Kulmanov, Yasmeen Hashish, Vladimir B. Bajic, Eva Goncalves-Serra, Nadia Schoenmakers, Georgios V. Gkoutos, Paul N. Schofield, Robert Hoehndorf
17 Apr 2017
→ doi: 10.1371/journal.pcbi.1005500   ↓

Selected conferences proceedings and posters

Complete list: https://openrisknet.org/library/

Tutorials

Selected tutorials

RevK Pharmacokinetics OpenRiskNet Case study using Jaqpot web modelling platform
Philip Doganis
15 Oct 2018

→ Video
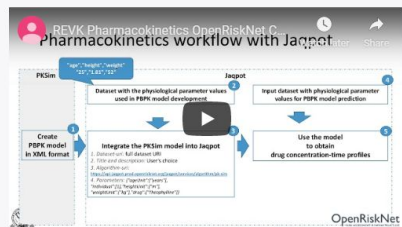
Related services:
Jaqpot GUI
Jaqpot API

Target audience: Risk assessors, Researchers, OpenRiskNet stakeholders, Data modellers
Open access: yes
Licence: Attribution-NonCommercial-ShareAlike 4.0 International (CC BY-NC-SA 4.0)
Organisations involved: NTUA

Model RX OpenRiskNet - Case study using Jaqpot web modelling platform
Philip Doganis
15 Oct 2018
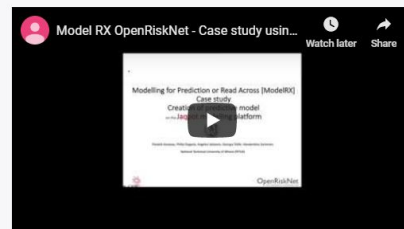
Related services:
Jaqpot GUI
Jaqpot API

Target audience: Risk assessors, Researchers, OpenRiskNet stakeholders, Data modellers
Open access: yes
Licence: Attribution-NonCommercial-ShareAlike 4.0 International (CC BY-NC-SA 4.0)
Organisations involved: NTUA

Workflow: Access TG-GATEs data for seleted compounds, select differentially expressed genes and identifier relevant pathways
Thomas Exner
13 Sep 2018

→ Workflow

Abstract:
Example workflow based on OpenRiskNet tools - Pathway identification workflow related to DataCure and AOPlink case studies. This notebook downloads TG-Gates data of 4 compounds and selects genes overexpressed in all sample. The Affymetrix probe sets are then translated into Ensembl gene identifiers using the BridgeDB service and pathways associated with the genes are identified using the WikiPathways service.

Related services:
BridgeDB identifier mapping service
EdelweissData serving ToxCast, ToxRefDB and TG-GATEs data
BridgeDb identifier mapping service (variety of species)
Jupyter Notebooks

Tutorials OpenRiskNet public website
30 Oct 2018

Abstract:
This document is addressed to OpenRiskNet and associated partners. Version 1 contains the following topics: How do I access the admin interface of the OpenRiskNet website?, How do I add and describe a new publication, training material or other resources?, How do I add and describe my services? and How do I add and describe a new event?

Webinar recordings

Webinar

OpenRiskNet   RISK ASSESSMENT E-INFRASTRUCTURE

www.openrisknet.org

Reports

Final definition of case studies (Deliverable 1.3) — Downloads 30, Views 55
Initial API version provided to providers of services (Deliverable 2.2) — 31, 48
Report of the Service Integration with OpenRiskNet - Initial Deployment... — 31, 47
Initial version of data management plan (Deliverable 3.1) — 22, 47
First report on the management process (Deliverable 5.1) — 29, 46
Development infrastructure online (Deliverable 2.1) — 22, 42
First documentation of the core e-infrastructure (Deliverable 3.2) — 18, 38
Report on Re-Identification Risks and Private by Design Risk Management... — 19, 35
Dissemination & Training Activities - Intermediate Report (Deliverable 3.4) — 17, 35
Report on deployment of virtual infrastructures with service discovery and... — 20, 34
Fully functional support infrastructure (Deliverable 3.3) — 15, 28
Report on requirements analysis and recommendations for WP2-4 (Deliverable... — 9, 28
Associated partner program is established (Deliverable 1.2) — 8, 28
Final API available for internal and external service providers (Deliverable 2.4) — 14, 26
Report of the Service Integration with OpenRiskNet (Intermediate Report)... — 10, 24
Compute and data federation (Deliverable 2.5) — 13, 14

■ Downloads   ■ Views

zenodo

OpenAIRE EXPLORE

SEARCH

OpenRiskNet

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

PROJECT   EC   OPEN ACCESS MANDATE FOR PUBLICATIONS AND RESEARCH DATA

Funding: H2020 | RIA
Start Date: 2016-12-01
End Date: 2019-11-30
Organization: Johannes Gutenberg University of Mainz | University of Birmingham | Fraunhofer | UM | UM | UvA | UvA | NTUA | MUI | IM | EwC | Uppsala University
Detailed project information (CORDIS) →

Publications (31) +
Research Data (1) +
Software (0) +
Other Research Products (2) +
Statistics +
Metrics +

OpenRiskNet Library:
https://openrisknet.org/library/

Final definition of case studies (Deliverable 1.3)   Report
Jennings, Paul; Exner, Thomas; Farcal, Lucian; Oki, Noffisat; Sarimveis, Harry; Doganis, Philip; Jennen, Danyel; Geerke, Daan; Willighagen, Egon; Bois, Frederic; Rautenberg, Micha; Dudgeon, Tim; Hardy, Barry
7 Nov 2018
→ doi: 10.5281/zenodo.1479127

Abstract:
OpenRiskNet case studies are used to test and evaluate solutions provided by the project to the predictive toxicology and risk assessment community, especially regarding the usability of the developed Application Programming Interfaces (APIs) and the interoperability layer. These case studies will demonstrate the capabilities to satisfy the requirements of the different stakeholder groups, including researchers, risk assessors and regulators and present real-world applications such as systems biology approaches for grouping compounds, read-across applications using chemical and biological similarity, and identifying areas of concern based on in vitro and in silico approaches for compounds lacking any previous knowledge from animal experiments (ab initio case).

Publisher: OpenRiskNet
Target audience: Risk assessors, Researchers, Nanosafety community, OpenRiskNet stakeholders, Regulators
Open access: yes
Licence: Attribution-ShareAlike 4.0 International (CC BY-SA 4.0)
Organisations involved: EwC, JSU, UM, NTUA, VU, IM, INERIS

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Public communication, News articles and blog posts

OpenRiskNet Library: https://openrisknet.org/library/

OpenRiskNet website News section:
https://openrisknet.org/news/

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Posts focused on case studies and demos

OpenRiskNet case studies enter final, test phase

31 January 2019

OpenRiskNet's work on case studies is entering the final phase with the focus on demonstrating infrastructure capabilities and on testing different risk assessment scenarios. The case studies provide examples and prototypes for solutions provided to the predictive toxicology and risk assessment community and demonstrate usage of the developed APIs and the interoperability features to build integrated workflows.

- DataCure - Data curation and creation of pre-reasoned datasets and searching
- ModelRX - Modelling for Prediction or Read Across
- SysGroup - A systems biology approach for grouping compounds
- MetaP- Metabolism Prediction
- AOPLink - Identification and Linking of Data related to AOPWiki
- TGX - Toxicogenomics-based prediction and mechanism identification
- RevK - Reverse dosimetry and PBPK prediction
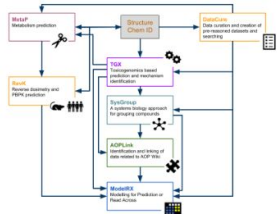
These cases also demonstrate how OpenRiskNet offers customised approaches for the different stakeholder groups (e.g., researchers, risk assessors and regulators) and provides fit-for-purpose services and solutions to real-world applications (e.g., systems biology approaches for grouping compounds; read-across applications using chemical and biological similarity).

Users are invited to become familiar with the OpenRiskNet concept before using its services. Please see **Webinars recording** and consult the **case studies description** that point out the services available and specific training materials. Over next few months, live demonstrations will be organised through public webinars to allow users to interact with OpenRiskNet service-providers.

Data curation workflows using OpenRiskNet approach ready for demonstration

18 March 2019

In the process of utilising the analysis tools available in the OpenRiskNet e-infrastructure, data needs to be accessed from different sources and various formats. Thus, the users should be able to access different data sources and specific entries. This are then being curated using an OpenRiskNet service and re-submitted to the data source.

Within DataCure case study, we aimed to establish a process for data curation and annotation that makes use of APIs and semantic annotations for a more systematic and reproducible data curation workflow. The development of semantic annotations and API definition for selected databases are also desired.

To achieve these, OpenRiskNet developed resources that can make use of APIs as much as possible and eliminate the need for manual file sharing. In addition workflows that provide examples of useful data for toxicogenomic data analysis will be developed.

This case study serves also as the entry point of curation of data sources to be used by the other case studies.

The technical implementation involved several steps related to the probability of data using Edelweissdata Explorer as **data source**, the data extraction in workflow, **data searching** using workflow that employ text **reasoning** done through the provision of workflows stored in Explorer as **submission to data source** where the curated datasets may be re-used.

To learn more on how this works in practice, you are invited to Please see more details on the webinar and register here.

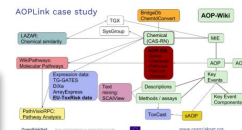## How to identify and link of data related to AOPWiki to support the Adverse Outcome Pathway approach

22 March 2019

The Adverse Outcome Pathway (**AOP**) concept has been introduced to support risk assessment [1]. An AOP comprise a number of biological events: a molecular initiating event (**MIE**) is followed by one or more key events (**KEs**), leading to the adverse outcome (**AO**). The AOPWiki [2] is a collaborative platform to exchange AOP-related knowledge.

The use of AOPs for regulatory purposes requires detailed validation and linking to existing knowledge [3; 4]. Part of the development of AOPs is the search for data that supports the occurrence and biological plausibility of KEs and their relationships (**KERs**). This data can be found in literature and increasingly in databases.

AOPlink case study developed within OpenRiskNet framework, focuses on establishing links between AOPs and data that supports a particular AOP. This will allow finding AOPs related to experimental data, and finding data related to a particular AOP.
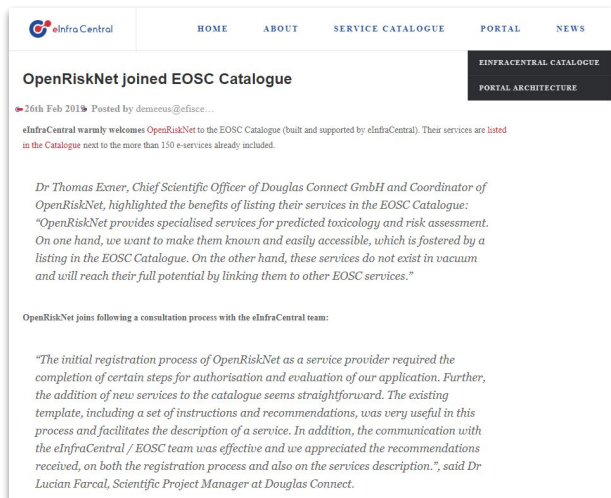
The federation of computing and data resources between the OpenRiskNet e-infrastructure and public computational and data resources has now been demonstrated

31 May 2019

The OpenRiskNet Consortium develops the OpenRiskNet e-infrastructure for the harmonisation and improved interoperability of data and software tools in the area of predictive toxicology and risk assessment. It aims to combine interoperable web services providing data or analysis, processing and modelling tools communicating over well-defined and harmonised application programming interfaces (APIs), supplemented by a semantic interoperability layer added to every service to describe the functionality whilst guaranteeing the technical and semantic interoperability.

An important task in the project, related also to the TGX case study, involved the federation of compute and data resources between the OpenRiskNet e-infrastructure and external resources. The reference environment has been designed to be capable of handling the majority of requirements for users wishes to deploy and run services. However specific situations demand solutions where either the computation, the data or both reside outside the OpenRiskNet e-infrastructure.

OpenRiskNet website News section:
https://openrisknet.org/news/

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Interactions with other EU e-infrastructure initiatives

- **eInfraCentral**: disseminate OpenRiskNet platform (or individual services) to a larger audience and be able to compare and connect with very similar services
- **OpenAIRE**: common philosophy on open source, open access and open data.
- **ELIXIR**: Toxicology and risk assessment were recently accepted as an ELIXIR community due to an application almost completely driven by OpenRiskNet partners.
- **ELIXIR's Training Portal**: https://tess.elixir-europe.org/content_providers/openrisknet
- **EU NanoSafety Cluster / NanoCommons**: nanosafety community is envisioned as one of the main beneficiaries of the OpenRiskNet services

Interactions with eInfraCentral and EOSC

OpenRiskNet joined EOSC Catalogue
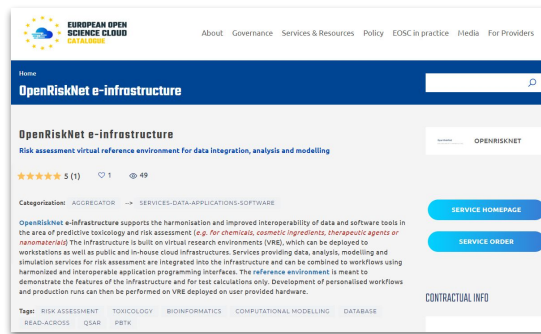
🗓 26th Feb 2019 Posted by demeeus@efisce...

eInfraCentral warmly welcomes OpenRiskNet to the EOSC Catalogue (built and supported by eInfraCentral). Their services are listed in the Catalogue next to the more than 150 e-services already included.

Dr Thomas Exner, Chief Scientific Officer of Douglas Connect GmbH and Coordinator of OpenRiskNet, highlighted the benefits of listing their services in the EOSC Catalogue: "OpenRiskNet provides specialised services for predicted toxicology and risk assessment. On one hand, we want to make them known and easily accessible, which is fostered by a listing in the EOSC Catalogue. On the other hand, these services do not exist in vacuum and will reach their full potential by linking them to other EOSC services."

OpenRiskNet joins following a consultation process with the eInfraCentral team:

"The initial registration process of OpenRiskNet as a service provider required the completion of certain steps for authorisation and evaluation of our application. Further, the addition of new services to the catalogue seems straightforward. The existing template, including a set of instructions and recommendations, was very useful in this process and facilitates the description of a service. In addition, the communication with the eInfraCentral / EOSC team was effective and we appreciated the recommendations received, on both the registration process and also on the services description.", said Dr Lucian Farcal, Scientific Project Manager at Douglas Connect.

Jaqpot
Generate, store and share predictive statistical and machine learning models

Lazar
Toxicity predictions

Squonk Computational Notebook
Computation research made simple and reproducible

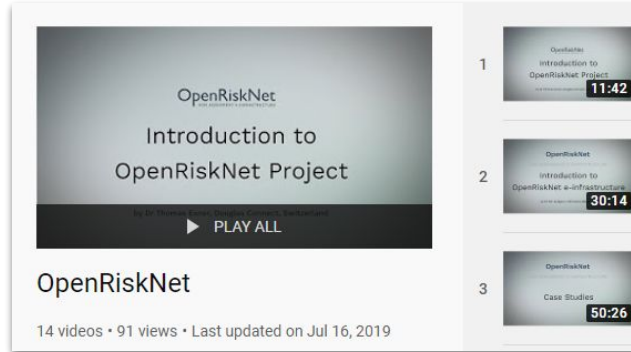**Participation at EOSC events** (posters and introduction to OpenRiskNet):

- **EOSC-hub Week**, 10 – 12 Apr 2019 / Prague, CZ
- **Building EOSC through the H2020 projects current status and future directions**, 9 – 10 Sep 2019 / Brussels, BE
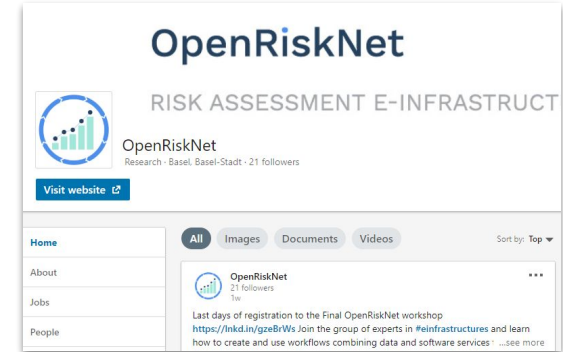
Social Media

Website analytics

Data Management Plan (DMP)

Deliverable 3.6 Final data management, maintenance and sustainability plan
https://docs.google.com/document/d/1Ag3e3gAFDix-WIdfKEZT_tODC8Mj9ILkIPqXOVGmKns/edit#

Data Management Plan

General and specific information (e.g. for diXa, BridgeDb, WikiPathways, AOP-Wiki and ToxCast) are provided on the following areas:

- Data summary
  - Purpose of the data collection
  - Relation to the objectives of the project
  - Types and formats of data
  - Reuse of data
  - Origin of the data
  - Expected size of the data
  - Utility of data and models
- FAIR data
  - Making data findable, including provisions for metadata
  - Making data openly accessible
  - Making data interoperable
  - Increase data re-use (through clarifying licenses)
- Allocation of resources
- Data security
- Ethical aspects (incl. Deliverable 6.7, final DPO report)

OpenRiskNet (Horizon 2020 DMP)

7/9

approx. 45% of available space used (max 10 pages)

| Plan details | **Initial DMP** | Detailed DMP | Final review DMP | Share | Export |

1. Data summary (1 question, 1 answered) +

2. FAIR data (4 questions, 4 answered) +

3. Allocation of resources (1 question, 0 answered) +

4. Data security (1 question, 1 answered) +

5. Ethical aspects (1 question, 1 answered) +

6. Other (1 question, 0 answered) +

Plan for the Exploitation and Dissemination of Results (PEDR)

PEDR version 3
https://docs.google.com/document/d/18TrkUcPtDzPdY5TpCrMjKkOXcH0tF_yNJuu0r_0ICLE/edit#

Plan for the Exploitation and Dissemination of Results (PEDR)

OpenRiskNet dissemination plan

- Dissemination and communication activities
- Dissemination performance metrics
- Reporting, tracking and sharing of dissemination activities
- Funding allocated for Dissemination and Communication activities

OpenRiskNet exploitation plan

- Virtual Organisation
- Sustainability plan
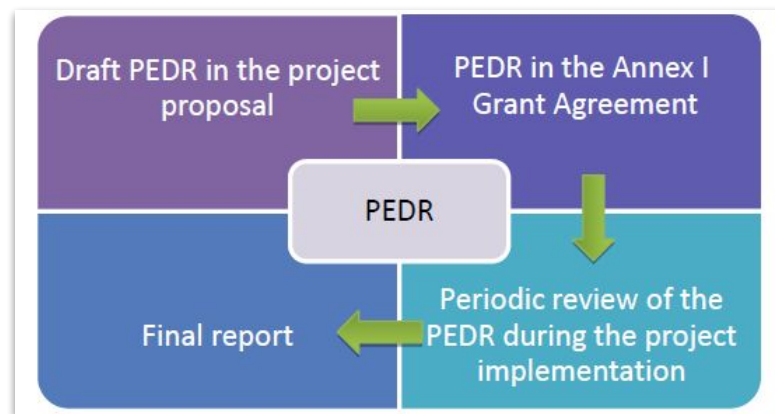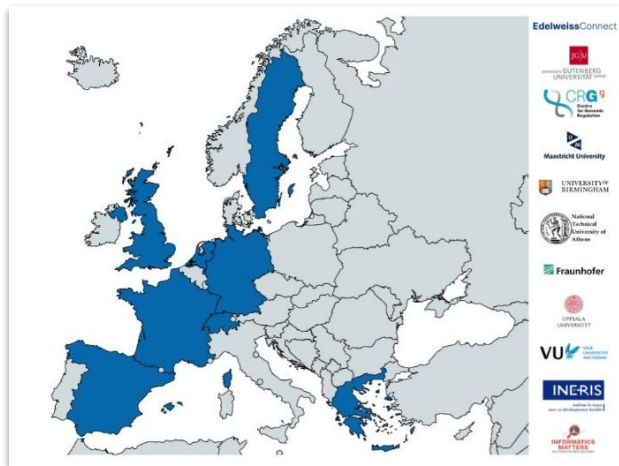
Sustainability

- Positioning OpenRiskNet as a major European provider of e-services for the toxicology community
  - Continuation in NanoCommons
  - Infrastructure in EU research projects

- Establishing toxicology and risk assessment as a major pan-European community with specific infrastructure needs
  - Listing on EOSC
  - Becoming a use case in EOSC-life
  - Collaborating with ENVRI
  - Trying to become part of a consortium of the remaining infrastructure calls (as a use case)

- Establishing OpenRiskNet as a place to offer and purchase data, predictive toxicology and risk assessment services
  - Service Model
  - Software Solution Consortium
  - Membership Model
  - Marketplace platform

Is it too early for this despite the good feedback we got from commercial service providers?

Acknowledgements

OpenRiskNet (Grant Agreement 731075) is a project funded by the European Commission within Horizon 2020 Programme

Project partners:

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