OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE

Deliverable Report D3.4

Dissemination & Training Activities (Intermediate Report)

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

Project Number 731075

www.openrisknet.org

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SUMMARY

This report describes the dissemination and training activities undertaken by the OpenRiskNet partners in the first half of the project. These activities were gathered formally within WP3 (Training, Support and Dissemination) but they cover aspects related to all WPs. Details and links to the various activities developed in the first half of the project were included, e.g. organisation of workshops, training events and hackathons, participation at conferences and workshops, peer-review publications, tutorials, public communication activities, the project website and visual identity development as well as the interactions initiated with other EU initiatives. The main dissemination activities related to OpenRiskNet are summarised on the project website at: https://openrisknet.org/library/

The report, follows the agreed Plan for the Exploitation and Dissemination of Results (PEDR) achieved at M6 (Milestone 1). This plan is used by the OpenRiskNet members as a basis for their dissemination activities and exploitation strategies.

INTRODUCTION

To foster the worldwide adoption of OpenRiskNet, a wide range of dissemination and networking activities (training sessions, workshops and hackathons) were executed with further iterations planned for the future. These activities were/are guiding also the definition of project priorities for sustaining a European risk assessment e-infrastructure and ensure direct exposure to the user communities. The dissemination activities have the following main objectives:

- Effective communication to the broader community in order to generate interest from organisations in using the OpenRiskNet infrastructure for predictive toxicology;
- Promote best practices and standards in data and knowledge management;
- Promote best practices and standards for interoperability between predictive toxicology, chemical and biological resources and services, and further the application of predictive toxicology methods in risk assessment;
- Disseminate information in order to arouse the interest of suppliers and developers in plugging additional products and services into the OpenRiskNet infrastructure;
- Develop close interactions with user communities and organisations with business needs for using the OpenRiskNet infrastructure and incorporating it into their product development and risk assessment activities.

These activities were gathered formally within WP3 (Training, Support and Dissemination) but they cover aspects related to all WPs, on technical, scientific and management matters. Also, a list of performance metrics for the dissemination and training activities were established in the project description. The list of metrics is presented in the first column of **Table 1.** The second column of the same table summarises the activities that were accomplished during the first half of the project and shows that all metrics for the mid-point of the project have been completely fulfilled.

The focus thus far has been to first announce the goals of the project and, as work progressed, to communicate the outcomes of the OpenRiskNet e-infrastructure in order to build consensus among stakeholders. These activities, mainly focused on the main target audiences of the project, represented by its end users (members of academia, industry, risk assessors and regulators), as well as by the developers (tools developers, data managers, infrastructure providers). Therefore, the envisaged dissemination and training activities target these communities of stakeholders.

Table 1. Performance metrics according to the project description related to dissemination and training activities

Metric	State until M18
Number of training workshops and hackathons: • >= 2 (until M18) • >= 5 (until M36)	Four training events, hackathons and workshops have been organised or supported until M18. Internal events: 1. API workshop, Mainz, Germany, January 2017 2. Hackathon session, Uppsala, Sweden, September 2017 External events:

	3. NetFlow workshop, Barcelona, Spain, September 2017 4. Training & Hackathon sessions at OpenTox Euro Conference, Basel Switzerland, November 2017
Acceptance of support facilities	The support functions for OpenRiskNet are functional and available, consisting of a helpdesk[1], a wiki[2], and an issue tracker[3] (see Deliverable 3.3).
Positive feedback from external participants at the workshops and hackathons	External participants at the hackathons (e.g. organised within OpenTox Conference 2017, Nextflow workshop) showed great interest in the biokinetics modelling capabilities offered through Jaqpot's API that provide functionality from the PKSim open-source software, as well as in new approaches to endocrine disruptor prediction improvement through utilisation of new database data and *in silico* or integrated *in silico-in vitro* approaches. Similarly, the participants had the opportunity to learn and use different applications or services (e.g. Jenkins, Squonk, CPSign, Nextflow, MDStudio) and actively interact with the tool developers.
Active participation in conferences and meetings • >= 5 (until M18) • >= 10 (until M36)	OpenRiskNet partners participated in 9 conferences or other events, with presentations or posters (complete list is given below).

Another achievement during this period was the preparation and agreement (Milestone 1 at M6) by the consortium on the OpenRiskNet Plan for the Exploitation and Dissemination of Results (PEDR), aiming to support and provide a basis for the OpenRiskNet members for their dissemination activities and exploitation strategies. This plan is currently followed and it will be updated if required, based on the latest developments and achievements in the project. The current Deliverable 3.4 is a follow-up action of the agreed PEDR and, therefore includes updates and achievements related to the dissemination and training activities performed by the OpenRiskNet members.

The current report includes details and links to the various activities developed in the first half of the project, focusing on the organisation of workshops, training events and hackathons, participation in conferences and workshops, publications, available tutorials, public communication activities, the project website and visual identity development, as well as the interactions established with other EU e-infrastructure initiatives like OpenAIRE, ELIXIR and eInfraCentral.

Additionally, tools like Zenodo / OpenAIRE or Twitter (#openrisknet) were used by project members to document and/or to promote the activities of OpenRiskNet.

[1] https://openrisknet.freshdesk.com
[2] https://github.com/OpenRiskNet/home/wiki
[3] https://github.com/OpenRiskNet/home/issues

Dissemination and training activities

Organisation of workshops, trainings and hackathons

During months 1-18, OpenRiskNet partners engaged in hackathons, focused to work on areas of interest, and in training sessions, aimed to provide training to participants about specific OpenRiskNet tools and infrastructure. Activities were aimed either internally, to promote development and collaborative work or externally, to interact with the community and receive feedback about current status and requirements, and also to calibrate future OpenRiskNet plans.

First OpenRiskNet API workshop, Mainz, Germany (16-17 January 2017)

Background

This internal workshop was related to the tasks on API specification and semantic interoperability and delivery of the initial API version. The outcomes of the meeting were included in the public Deliverable 2.2.

Objectives

The OpenRiskNet team gathered to discuss the APIs, starting from the current status available at partners and extending on their specifications, documentation formats, use cases and services to be integrated, service discovery and reach agreement on techniques and tools that to be used within OpenRiskNet. The detailed program is included in the Annex.

Nextflow Workshop “Reproducible *in silico* genomics”, Barcelona, Spain (14-15 September 2017)

Background

OpenRiskNet supported this Nextflow event[4] jointly with other initiatives. Nextflow is a novel pipeline development tool developed by the Centre for Genomic Regulation CRG (partner in OpenRisKnet), emerging as an efficient solution to the reproducibility dilemma in omics analyses.

Objectives

The aim was to bring together Nextflow developers, workflow experts and bio-informaticians to discuss the current state of Nextflow technology, the latest developments and the open questions to tackle the problem of reproducible -omics analyses. Best practices were introduced using practical examples on how to handle production of large-scale genomic applications for precision medicine.

[4] http://www.crg.eu/en/event/coursescrg-nextflow-reproducible-silico-genomics

OpenRiskNet Hackathon, Uppsala, Sweden (25-26 September 2017)

Background

The hackathon[5] was organised as a follow up to the previous API meeting in Mainz, and focused on microservices development with a concentration on Kubernetes/OpenShift and how a CICD system can be established within the OpenRiskNet project.

Objectives

The hackathon aimed to improve OpenRiskNet partners' competence on cloud technologies, such as containers (docker), container orchestration tools and discussed options of what is needed to create or adapt applications that run and interoperate within an OpenRiskNet virtual research environment (VRE). We also introduced and work practically with different technologies and systems (including Docker, Kubernetes, Openshift, Continuous integration/testing/deployment (CICD), Single Sign On (SSO)) working towards getting more tools ready for running in the emerging OpenRiskNet framework, while also enabling discussions on API and interoperability. Another topic addressed was the infrastructure options for the deployment of OpenRiskNet. The detailed program is included in the Annex.

OpenRiskNet Training & Hackathon, Basel, Switzerland, 20-21 November 2017

Background

The OpenRisknet consortium organised training and hackathon sessions[6] at the OpenTox Euro 2017 Conference. The OpenTox Association runs a series of conferences that take place on an annual basis in Europe, Asia and the US, bringing together experts in the field of Open Toxicology.

Objectives

The aim was to present the OpenRiskNet approach and tools and engage with the greater community. The parallel sessions covered topics on modelling services, workflow management systems and ontology annotation of datasets, QSAR and NanoQSAR predictive modelling, endocrine disruptor data sources and predictions. The concept of semantic annotation of services was also presented and applied to a biokinetics modelling tool. The detailed program is included in the Annex.

[5] https://pharmb.io/blog/orn-workshop-2017/
[6] http://www.opentox.net/events/opentox-euro-2017/training-and-hackathon

Participation at conferences and workshops

In the first 18 months, relevant events were attended by the OpenRiskNet members, promoting the project concepts and developments. The complete list of events is included in **Table 2**, while the highlights of presentations and posters presented at different events is available in the Library[7] on the project website. Moreover, participation in future events is already planned until the end of 2018 (**Table 3**).

Table 2. Summary of the participation at conferences and workshops by OpenRiskNet members

Title/Topic	Type	Authors	Event
OpenRiskNet, an open e-infrastructure to support data sharing, knowledge integration and in silico analysis and modelling in risk assessment[8]	Poster	Exner T, Dokler J, Bachler D, Farcal L, Evelo C, Willighagen E, Jacobs M, Doganis P, Sarimveis H, Lynch I, Kramer S, Notredame C, Jennen D, Gkoutos G, Spjuth S, Jennings P, Dudgeon T, Bois F, Hardy B	SOT 2018 (Society of Toxicology 57th Annual Meeting and ToxExpo), 11-15 March 2018, San Antonio (USA)
If we all jump together, could we make the earth move?	Oral presentation - Keynote Talk	Chris Evelo (MU)	OpenTox Euro 2017, 21-23 November 2017, Basel (Switzerland)
The OpenRiskNet Project	Oral presentation	Thomas Exner, (Douglas Connect GmbH, Switzerland)	
Towards Semantic Interoperability of Publicly Available Data	Oral presentation	Thomas Exner, (Douglas Connect GmbH, Switzerland)	
Characterisation of intrinsic and extrinsic nanomaterial characteristics: the need for relevant exposure media supplemented with appropriate biomolecules	Oral presentation	Iseult Lynch (UoB)	
Enriching Key Events in Adverse Outcome Pathways with links to biomolecular databases to allow experimental data analysis for regulatory risk assessment	Oral presentation	Marvin Martens (MU)	

[7] https://openrisknet.org/library/
[8] https://doi.org/10.5281/zenodo.1199287

Data-intensive applications on cloud computing resources: Applications in life sciences[9]	Oral presentation	Ola Spjuth (UU)	de.NBI 2017 symposium 'The Future Development of Bioinformatics in Germany and Europe', Bielefeld, 23 October 2017, Bielefeld (Germany)
RDKit software	Participation at the workshop	Daniel Bachler (DC), Tim Dudgeon (IM)	RDKit User Group Meeting, 20-21 September 2017, Berlin (Germany)
Data-intensive bioinformatics on HPC and Cloud[10]	Oral presentation	Ola Spjuth (UU)	Big Data Training School for Life Sciences, 18-22 September 2017, Uppsala (Sweden)
Nextflow for chemistry - crossing the divide[11]	Oral presentation	Tim Dudgeon, (IM)	Nextflow (Reproducible in silico Genomics), 14-15 September 2017, Barcelona (Spain)
An Open Source web platform for modelling and model publishing integrated into a Safety Assessment e-infrastructure[12]	Poster	P. Doganis, G. Tsiliki, C. Chomenidis, A. Valsamis, E. Anagnostopoulou, & H. Sarimveis (NTUA)	OSFAIR2017, September 6-8, 2017, Athens, Greece
Toward Semantic Interoperability of Public Available Data Sources[13]	Oral presentation	Thomas Exner, (DC)	OpenTox USA (12-13 July 2017, Durham, USA)
The future of regulatory toxicity assessment[14]	Poster	Marvin Martens, Chris Evelo, Egon Willighagen (MU)	byteMAL Conference (Bioinformatics for Young inTernational researchers Expo: Maastricht-Aachen-Liège, June 2017, Maastricht, The Netherlands)

9 https://www.slideshare.net/ospjuth/dataintensive-applications-on-cloud-computing-resources-applications-in-life-sciences

10 https://www.slideshare.net/ospjuth/dataintensive-bioinformatics-on-hpc-and-cloud

11 https://openrisknet.org/docs/Nextflow-Workshop-2017_v2.pdf

12 https://f1000research.com/posters/6-1865

13 https://doi.org/10.5281/zenodo.831444

14 https://doi.org/10.6084/m9.figshare.5331517.v1

Table 3. Planned participation at conferences and workshops by OpenRiskNet members in the next period of the project

Title/Topic	Type	Authors	Event
How to overcome the data gaps in nanomaterial risk assessment	Oral presentation	Exner T (DC)	Nano Korea 2018, 10-13 July 2018 (Korea)
Introducing WikiPathways as a data-source to support Adverse Outcome Pathways for regulatory risk assessment of chemicals	Poster	Martens M., Willighagen E, Evelo C (UM)	EUROTOX 2018, 2-5 September 2018, Brussels (Belgium)
Meta-analysis for genotoxicity prediction using data from multiple human in vitro cell models	Poster	Bayjanov J. R., Kleinjans J., Jennen D. (UM)	
OpenRiskNet, an open e-infrastructure to support data sharing, knowledge integration and in silico analysis and modelling in risk assessment	Poster	Exner T, Dokler J, Bachler D, Farcal L, Evelo C, Willighagen E, Jennen D, Jacobs M, Doganis P, Sarimveis H, Lynch I, Gkoutos G, Kramer S, Notredame C, Spjuth S, Jennings P, Dudgeon T, Bois F, Hardy B	
eNanoMapper solutions for FAIR sharing of nanosafety data	Oral presentation	Willighagen E (UM)	NanoTox 2018, 19-21 September 2018, Neus (Germany)
Towards intelligent drug safety predictions	Oral presentation	Ola Spjuth (UU)	Swedish Bioinformatics Workshop, 25-26 October 2018, Örebro (Sweden)

An important next event supported by OpenRiskNet (in collaboration with NanoCommons) is the OpenTox Euro 2018[15], organised in Athens (Greece) between 8-11 October. The theme of the conference is "*Bridging the gap between experimental and computational work in safety and risk assessment*" and covers topics on the emerging methods in safety assessment, the use of integrated testing strategies and integrated experimental and data workflows.

[15] http://www.opentox.net/events/opentox-euro-2018

Peer-reviewed publications

The following Open Access peer-review scientific articles were published within the first 18 months of the project:

- Boudellioua I, Mahamad Razali RB, Kulmanov M, Hashish Y, Bajic VB, Goncalves-Serra E, Schoenmakers N, Gkoutos GV, Schofield PN, Hoehndorf R, Semantic prioritization of novel causative genomic variants, PLoS Comput Biol. 2017, 13(4):e1005500, April 2017. doi: 10.1371/journal.pcbi.1005500 (*Available also in OpenAIRE*)
- Lapins M, Arvidsson S; Lampa S, Berg A; Schaal W, Alvarsson J, Spjuth O, A confidence predictor for logD using conformal regression and a support-vector machine, J. Cheminformatics. 2018, 10:17 doi: 10.1186/s13321-018-0271-1

Tutorials

As the OpenRiskNet services and tools are developed and made available to users, a series of tutorials are prepared, as needed, to further support the developers as well as the users. These tutorials are presented together with the relevant services and included within their specific documentation.

The initial work on this task, includes the following tutorials and implementations related also to previous projects (i.e. eNanoMapper) and ongoing initiatives (i.e. NanoCommons).

- Adding ontology terms
  https://enanomapper.github.io/tutorials/Added%20ontology%20terms/
- Browsing the eNM ontology with BioPortal, AberOWL and Protégé
  https://enanomapper.github.io/tutorials/BrowseOntology/Tutorial%20browsing%20eNM%20ontology.html

Deployment clinics

A series of deployment sessions were organised dedicated in the first phase to the OpenRiskNet developers. The materials generated are publicly available[16] for further use by the service providers. So far, six sessions were organised:

1. OpenShift deployment
2. Deploying applications
3. Single Sign-On system
4. Persistence in OpenShift
5. Jaqpot service deployment

The technical details on these are included in Deliverable 2.3.

[16] https://drive.google.com/drive/u/0/folders/1A98zl9P0387ifTsI9w2QP0linGX6lTwq

Public communication

A series of communication activities, targeting also other type of audiences, were initiated. The aim is to reach out to specific communities of scientists (e.g. nanosafety scientists) or even to the general public. These activities included press releases, blog posts, announcements and news[17] on current activities and achievements. The communication activities undertaken to date are summarised in **Table 4**.

Table 4. Summary of public communication activities

Title/Topic	Type and date	Url
The OpenRiskNet Approach towards a Semantic Interoperability Layer - Part One: Problem Definition for Datasets	Blog post (17-Jan-2018)	https://openrisknet.org/news/blog-semantic-interoperability-201801
OpenRiskNet reveals concepts of harmonised APIs and semantic interoperability, provides first training units, and launches Associate Partner Program	Press Release (8-Dec-2017)	https://openrisknet.org/news/press-release-2017/
OpenRiskNet case studies to support data and tools integration from NanoSafety Cluster	NSC Newsletter Issue No. 10, Autumn 2017 (pg. 7) (2-Nov-2017)	http://www.nanosafetycluster.eu/uploads/files/NSC_Newsletter/NSC_Autumn2017_Bulletin.pdf
Horizon 2020 Research Success Story - A global harmonized basis for testing chemical safety	Interview and article for Euresearch.ch (Aug-2017)	https://www.euresearch.ch/fileadmin/redacteur/Media/OpenRiskNet_Success_Story_201708_high.pdf https://www.youtube.com/watch?v=-40OGH07PaQ&feature=youtu.be
Introduction to OpenRiskNet	NSC Newsletter Issue No. 9, Spring 2017 (pg. 15) (4-Apr-2017)	http://www.nanosafetycluster.eu/uploads/files/NSC_Newsletter/NanoSafety_Cluster_Newsletter_Issue_9_Spring_2017.pdf
OpenRiskNet Kicked off	Blog post (24-Jan-2017)	http://douglasconnect.com/blog/openrisknet-kicked

[17] https://openrisknet.org/news/

Project website and visual identity

The OpenRiskNet website (https://openrisknet.org/) was released in June 2017, to enable presentation of project work to its stakeholders (i.e. end users and developers), the scientific community and to the general public. The website contains general information on project objectives and partners, detailed information on the Associate Partner Programme and a list of the main dissemination activities. On the technical development side, the website provides information on case studies and associated use cases, but also the description of the stepwise API Design Concept adopted. **Figure 1** shows a screenshot of the OpenRiskNet home page.

The website format follows all the requirements established by the EC within the H2020 programme on public funding acknowledgments.

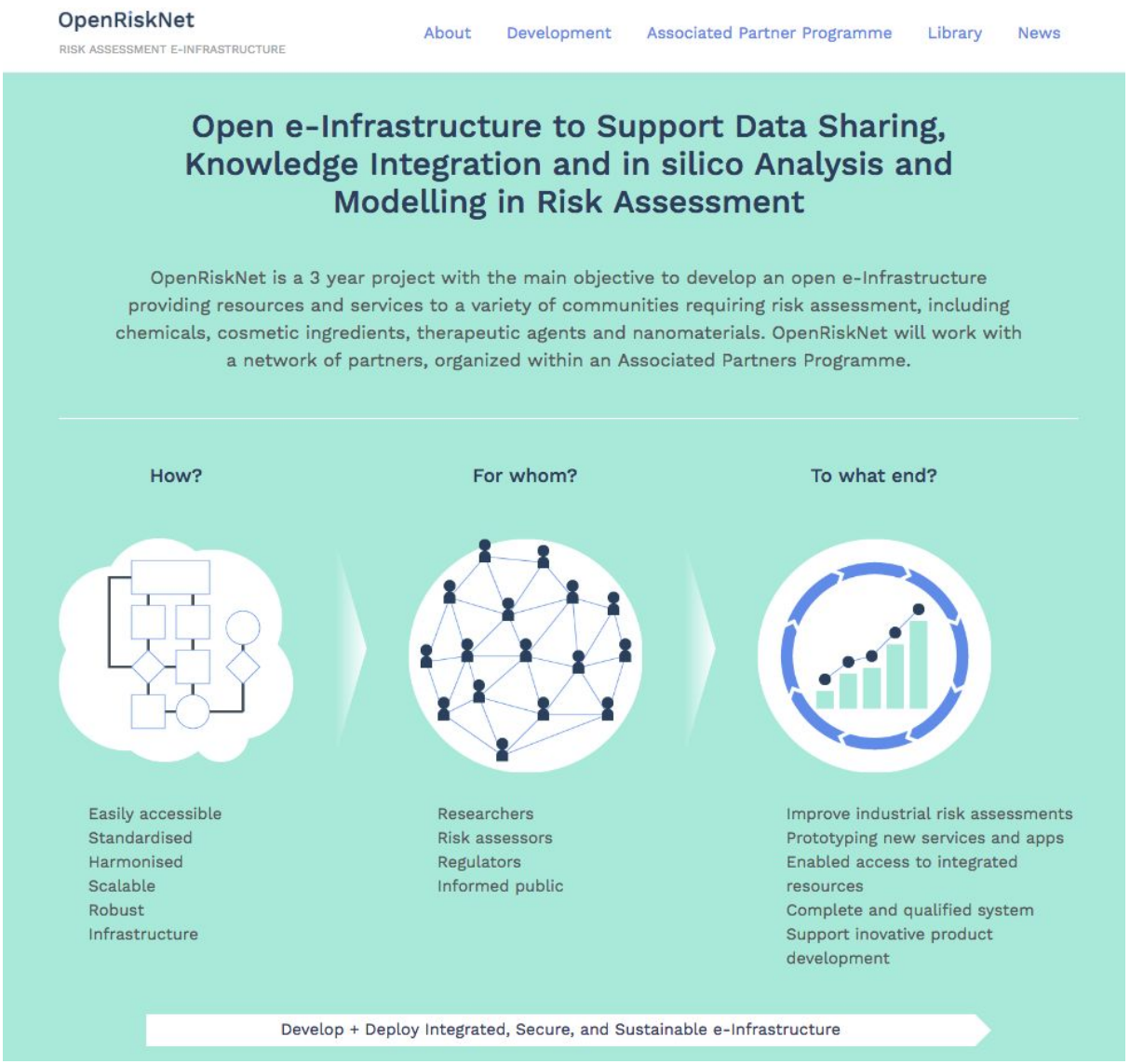

Figure 1. Screenshot of the OpenRiskNet home page

In parallel with the website preparation, additional dissemination items and materials were developed and implemented. Therefore, a set of different versions of project logo was created (see **Figure 2**) and used for different purposes, including the templates for the projects reports and presentations.

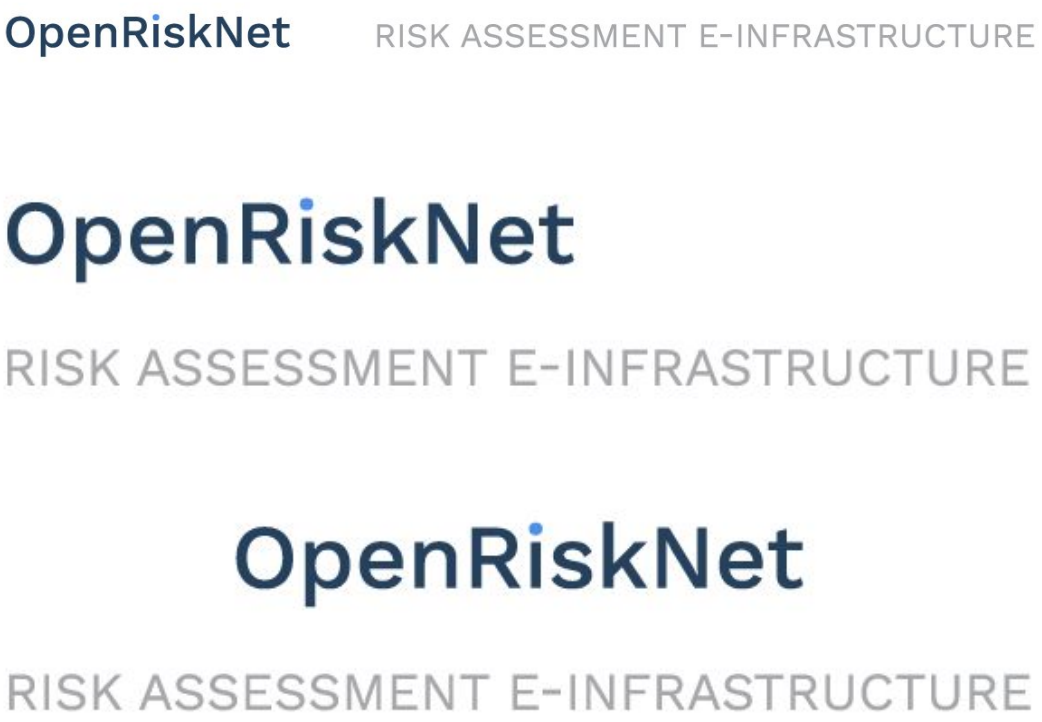

Figure 2. Different versions of OpenRiskNet logo

Interactions with EU e-infrastructure initiatives

eInfraCentral

In the context of the development of the European Open Science Cloud and following a request from the eInfraCentral coordination and support action[18], OpenRiskNet started a series of interactions with eInfraCentral, exchanging information on the objectives, requirements and further actions. The topics of the first indications included:

- An assessment of service management standards/framework to facilitate the decision making process of e-Infrastructures to adopt a standard or framework and a service management vocabulary put forward to allow for convergence to a common vocabulary;
- A pre-standard service description template to allow for structured service descriptions by e-Infrastructures and service (re)presentation templates;
- A harmonised and aggregated service catalogue populated already with more than 70 services and best practices and recommendations for effective service descriptions and representations.

This EU action will ensure that by 2020 a broader and more varied set of users discovers and accesses the existing and emerging e-Infrastructure capacity and e-Science Services. eInfraCentral aims to develop the EU's e-Infrastructure service catalogue gateway and extend the platform to services provided by other major e-Infrastructure service providers; therefore they invited also the OpenRiskNet infrastructure to join this collaborative effort.

As part of the EU e-infrastructure catalogue[19], OpenRiskNet would benefit by disseminating its platform (or individual services) to a larger audience and be able to compare and connect with very similar services. However, further contribution to the common platform should consider a few aspects on the specificity of the services (e.g. related mainly to toxicology, data modelling and risk assessment) and the specific targeted audience of OpenRiskNet. Further, aspects on the manual versus automatic updates of the information, the availability of APIs, the granularity of the catalogue, clustering of services and the service description template are under consideration and will be the subjects of further discussion and interactions.

The service description template provided by eInfraCentral contains the following main sections:

- Basic Service Information (e.g. service ID, URL, Provider, etc.);
- Service Classification Information (details on the service version, updates, TRLs, etc.);
- Service Support Information (any support information offered by the provider, including helpdesk, manuals, etc.);
- Service Contractual Information (terms of use, funding, price, etc.);
- Service Performance Information (details on service availability, reliability, other performance indicators).

[18] www.einfracentral.eu
[19] http://beta.einfracentral.eu/home

OpenAIRE

OpenAIRE's aim is to become the European scholarly communication hub providing its services to many European funders[20]. For this, it has built a network of Open Access repositories, archives and journals that support Open Access policies. It goes beyond the traditional publications aggregator by interconnecting entities related to scholarly communication (publications, research data, funding, people, organizations, data sources) allowing users to navigate alongside a rich information space graph and provides a wide range of services, from deposition to statistics. OpenRiskNet is using parts of the OpenAIRE infrastructure, especially Zenodo[21], the catch-all repository for EC funded research, for broad dissemination of the project reports (following the formal approval by the EC) as well as submitting project presentations and posters.

Due to the common philosophy (open source, open access and open data), a collaboration between OpenAIRE and OpenRiskNet was initiated, with a first highlight being the talk given by Alessia Bardi introducing the OpenAIRE services (Title: OpenAIRE services in support of "Open Science as-a-Service")[22] at OpenTox Euro 2017. During this event and additional virtual meetings, the specific requirements of the OpenRiskNet project and possible ways to link the structured data sources from toxicology research into the indexing services of OpenAIRE were discussed.

ELIXIR

ELIXIR unites Europe's leading life science organisations in managing and safeguarding the increasing volume of data being generated by publicly funded life sciences research. It coordinates, integrates and sustains bioinformatics resources across its member states[23]. Toxicology and risk assessment were recently accepted as an ELIXIR community due to an application almost completely driven by OpenRiskNet partners.

This will further strengthen the collaboration between ELIXIR and OpenRiskNet facilitated by the overlap of partners in both infrastructures.

EU NanoSafety Cluster - NanoCommons

The nanosafety community is envisioned as one of the main beneficiaries of the OpenRiskNet services. On the other hand, OpenRiskNet builds on developments resulting from nanosafety research and especially of the eNanoMapper project. Therefore, close collaboration is ongoing, which lead to OpenRiskNet becoming an associated project to the EU NanoSafety Cluster (NSC)[24], and will be continued and strengthened by knowledge exchange with the recently funded infrastructure project NanoCommons[25].

Within the interactions with the NSC, we are also investigating (as part of the NSC Workspace setup for this purpose) the features of the Common Dissemination Booster (CDB)[26], a service offered free of charge by the European Commission.

[20] https://www.openaire.eu/
[21] https://zenodo.org/
[22] http://www.opentox.net/events/opentox-euro-2017/OpenAIRE-services
[23] https://www.elixir-europe.org/
[24] https://www.nanosafetycluster.eu/
[25] www.nanocommons.eu
[26] https://www.cdbservices.eu/

CONCLUSION

During the first 18 months, OpenRiskNet partners actively undertook event organisation activities, in order to provide active training of OpenRiskNet tools and advance internal and external knowledge and also to disseminate results to the broader community of risk assessment researchers and professionals. The performance metrics assigned to monitor the progress have been met, demonstrating successful implementation of project plans.

As shown above, the OpenRiskNet consortium supported and was involved in the organisation of different community events, targeting different types of stakeholders, from developers to researchers and risk assessors.

Interactions with other EU e-infrastructures initiatives (e.g. eInfraCentral, OpenAIRE, ELIXIR and EU Nanosafety Cluster/NanoCommons) were established in order to ensure a broader dissemination of the OpenRisknet concepts and developments.

GLOSSARY

The list of terms or abbreviations, with the definitions, used in the context of OpenRiskNet project and the e-infrastructure development is available:

https://github.com/OpenRiskNet/home/wiki/Glossary

ANNEXES

Annex 1. Program of the API meeting (Mainz, Germany)

Monday 16.01.2017

09:30 Opening and Introduction - Andreas Karwath (JGU)

10:00 Use cases and case studies

- Use case presentation from *Danyel Jennen (UM)*

11:20 API presentations

- OpenTox API history - *Micha Rautenberg (JGU)*
- Conformal Prediction - *Staffan Arvidsson (UU)*
- eNanoMapper Substance APIs - *Egon Willighagen (UM)*
- eNanoMapper Modelling APIs - *Angelos Valsamis (NTUA)*
- Data APIs (ToxCast/ToxRefDB/OpenTGGates) - *Daniel Bachler (DC)*
- Squonk APIs - *Tim Dudgeon (IM)*

12:30 Lunch

14:00 Discussions on APIs

18:00 End first day

Tuesday 17.01.2017

09:00 Wrap up from first day & Goal setting

09:30 Initial design more complex use cases and API modifications

12:30 Lunch

13:30 Start afternoon session

16:00 End

Annex 2. Program of the OpenRiskNet Hackathon (Uppsala, Sweden)

Monday, September 25	
9:00- 9.30	Workshop start, overview, objective - *Ola Spjuth (UU)*
9.30-10.30	Cloud computing basics and KubeNow - *Marco Capuccini (UU)*
10.30-10.45	Coffee
10:45-12:00	Introduction to Docker, Kubernetes and OpenShift - *Tim Dudgeon (IM)*
12:00-13:00	Lunch
13:00-17:00	Hands-on with Docker, Kubernetes/OpenShift - *Jonathan Alvarsson (UU), Tim Dudgeon (IM)* and others
Tue Sept 26	
9:00-10:30	CICD in OpenShift. Intro + hands-on: How to build a service in ORN - *Tim Dudgeon (IM), Jonathan Alvarsson (UU)*
10.30-10.45	Coffee
10:45-12:00	Configuration, persistence and SSO - how to configure an app into its environment - *Tim Dudgeon (IM), Jonathan Alvarsson (UU)*
12:00-13:00	Lunch
13.00-15.00	API and semantic interoperability - *Daniel Bachler (DC)*
15.00-16.00	Hacking
16.00	Wrap-up

Annex 3. Program of the Training & Hackathon (Basel, Switzerland)

21 Nov 2017

PARALLEL TRAINING SESSIONS

11.00-13.00 ONTOLOGIES

Title: Semantic/ontologies
Type: Training
Duration: 120 min
Responsible(s): Egon Willighagen (UM)

Summary

- Short reminder on how to browse ontologies
- Introduction to the Jenkins build system, Slimmer and the eNanoMapper ontology
- Initial population of a general toxicology ontology
- Work on ISO terminology

Prior knowledge: not required

Resources

- Jenkins build server build server
- ontology GitHub repository
- ontology tests GitHub repository
- eNanoMapper ontology browsing tutorial

https://github.com/enanomapper/tutorials/blob/master/BrowseOntology/Tutorial%20browsing%20eNM%20ontology.md

11.00-12.00 NANOQSAR MODELLING

Title: NanoQSAR modelling (Jaqpot online platform)
Type: Training
Duration: 60 min
Responsible(s): Philip Doganis (NTUA)

Summary

Training aim: Provide a modeling experience on nanoQSAR in two directions: Users that wish an introduction to modeling tools will be able to create their first models using the user interface Jaqpot provides.
Expected outcomes: Provide a foundation course on online modeling to serve as basis for the hackathon and hands-on experience with tools.
Requirements: Understanding of QSAR concepts.

Resources

HYPERLINK
https://drive.google.com/drive/folders/10jmlKIo2cfCGDvStuNPc_u3sUDYtpL9q?usp=sharing

12.00-13.00 QSAR AND CONFORMAL PREDICTIONS

Title: QSAR and conformal predictions (CPSign, ModelingWeb)
Type: Training
Duration: 60 min
Responsible(s): Ola Spjuth (UU)

Summary

■ A short introduction to conformal prediction
■ A hands-on exercise with the CPSign program on command-line, allowing for training models and making predictions using conformal prediction with visualization/interpretation of important substructures
■ A demo of the current status of the web based services (ModelingWeb) wrapping CPSign and offering an API in OpenRiskNet

Resources

Documentation for CPSign -- http://cpsign-docs.genettasoft.com/
Files access:
https://drive.google.com/open?id=1soPPTx9xVcxWYoV069RlkWfScLfMtMB4

PARALLEL TRAINING SESSIONS

14.00-16.00 BIOKINETICS MODELLING

Title: Biokinetics modelling
Type: Training
Duration: 120 min
Responsible(s): Frederic Bois (INERIS) and Harry Sarimveis (NTUA)

Summary

■ **Aim:** understanding the use, form, inputs and outputs of physiologically based (PBPK) pharmacokinetic models.
■ **Expected outcome:** the participants should be able to attend usefully the next day hackathon.
■ **Requirements:** superficial reading of the bibliography given in the resources section below.

Agenda:

■ General presentation of PBPK models (F. Bois, 45 minutes)
■ Presentation of software applications for developing PBPK models. Customising PBPK to individual time-drug concentration data. Creating optimal drug dosage regimens (H. Sarimveis, 35 minutes)

Resources

About the software PKSim, see http://www.open-systems-pharmacology.org/ and documentation herein:
https://github.com/Open-Systems-Pharmacology/OSP-based-publications-and-content/issues?q=is%3Aopen+is%3Aissue+label%3AJournal
See for example the recent
https://github.com/Open-Systems-Pharmacology/OSP-based-publications-and-content/issues/104

14.00-16.00 WORKFLOW MANAGEMENT SYSTEMS

Title: Workflow management systems (nextflow, squonk)
Type: Training
Duration: 120 min
Responsible(s): Tim Dudgeon (IM), Cedric Notredame (CRG), Daan Geerke (VU) and Marc van Dijk (VU)

Summary
We will describe and demonstrate workflow tools that will be incorporated into the OpenRiskNet platform, and form a key aspect of the ways end users interact with the OpenRiskNet services. This will primarily be a demo of the tools involved and a discussion of how we plan to use and integrate these in OpenRiskNet, along with a limited opportunity to use these tools in a hands-on manner.
Agenda:
1. Introduction to the OpenRiskNet platform
2. Nextflow: orchestrating complex scientific workflows
3. Squonk Computational Notebook: a workflow tool for non-geeks
4. MDStudio: a microservice based workflow system

Resources
Nextflow (http://nextflow.io)
Nextflow enables scalable and reproducible scientific workflows using software containers. It allows the adaptation of pipelines written in the most common scripting languages. Its fluent DSL simplifies the implementation and the deployment of complex parallel and reactive workflows on clouds and clusters.
Squonk Computational Notebook (http://squonk.it)
A web based collaborative workflow building and execution environment, along with data visualisation and analysis capabilities. It includes the ability to easily plug in additional services through Docker images.
MDStudio
MDStudio deploys microservice based, scalable, reproducible and multi-user ready computational workflows at various levels of abstraction. Everything is a microservice: software, scripts, web services, databases, dedicated HPC pipelines and more. Using only a network connection to communicate, MDStudio microservices natively scale up and out on heterogeneous platforms providing a flexible means of creating workflows tailored to the requirements of a research team.

HACKATHON SESSIONS
16:30 - 17:30 BIOKINETICS HACKATHON

Title: Biokinetics modelling
Type: workshop/hackathon
Duration: 30 min introduction + 60 min hands-on
Responsible(s): Frederic Bois (INERIS) and Harry Sarimveis (NTUA)

Summary
The aim of this workshop is to create a biokinetics model using the PKSim software and then use ORN functionalities to expose the model as a service on the web.
During this workshop we will:
■ Show the basic functionalities of Jaqpot API and UI.
■ Guide the preparation of biokinetics models using the PKSim software.
■ Demonstrate how to use the Swagger documentation of JaqPot API to expose the model as a web service and use it for generating time-drug concentration profiles.

Resources
https://drive.google.com/drive/folders/1wGmqNYI8GnDL_orrE2JqPQAMauHStbPj

16:30 - 17:30 HACKATHON ON ESTROGENIC ACTIVITY DATA

Title: Estrogenic activity data for endocrine disruption predictions
Responsible(s): Thomas Exner (DC)
Type: Hackathon
Duration: 30 min introduction + 150 min hands-on

Summary

Endocrine disruption is of major regulatory importance. ECHA and EFSA are developing at the moment scientific guidance to enable endocrine disruptors to be identified (unfortunately not public available yet). FDA have created over the years valuable resources in form of the Endocrine Disruptor Knowledge Base (EDKB) and the Estrogenic Activity Database (EADB) and the estrogen and androgen receptors are important targets in EPA's ToxCast and Tox21.
The hackathon is meant to look at these data sources and different *in silico* and integrated *in silico-in vitro* approaches and identify areas in which especially the new FDA data in combination with other data sources could help to improve the existing methods.

Resources

- EDKB:https://www.fda.gov/ScienceResearch/BioinformaticsTools/EndocrineDisruptorKnowledgebase/default.htm
- EDKB paper: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3026379/
- EADB:https://www.fda.gov/ScienceResearch/BioinformaticsTools/EstrogenicActivityDatabaseEADB/default.htm
- EDKB paper: https://academic.oup.com/toxsci/article-lookup/doi/10.1093/toxsci/kft164
- US EPA Endocrine Disruptor Screening Program – The Pivot:https://cfpub.epa.gov/si/si_public_file_download.cfm?p_download_id=523453
- EDSP21 Dashboard: https://actor.epa.gov/edsp21/
- US National Toxicology Program: https://ntp.niehs.nih.gov/pubhealth/evalatm/test-method-evaluations/endocrine-disruptors/index.html
- ToxCast/Tox21: https://actor.epa.gov/dashboard/ and https://data.douglasconnect.com/
- FDA case study: https://dx.doi.org/10.1021/acs.chemrestox.5b00243

Tox21 models

- Overview: https://www.frontiersin.org/research-topics/2954/tox21-challenge-to-build-predictive-models-of-nuclear-receptor-and-stress-response-pathways-as-media#articles
- Ahmed's models: https://www.frontiersin.org/articles/10.3389/fenvs.2016.00002/full and http://ochem.eu/article/98009
- Nicole's models: https://pubs.acs.org/doi/abs/10.1021/acs.chemrestox.6b00347, https://pubs.acs.org/doi/abs/10.1021/acs.est.5b02641 and HYPERLINK https://www.endocrinescience.org/wp-content/uploads/2015/12/AmericanChemistry-EPA-Scientists-Working-PC-12-15.pdf

WEDNESDAY, 22 NOVEMBER 2017
08.30-11.00 **Continuation Data and API Hackathons**

Hands-on session on the topics introduced the day before