

OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE

Deliverable Report D3.5

Dissemination & Training Activities (Final Report)



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

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www.openrisknet.org

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Table of Contents

SUMMARY	5
INTRODUCTION	6
DISSEMINATION & TRAINING ACTIVITIES	9
Events	9
Organisation of webinars	9
Organisation of workshops, trainings and hackathons	13
Final OpenRiskNet Workshop: Creating powerful workflows combining data and software services demonstrated on risk assessment case studies	13
Participation at conferences and workshops	20
Resources and training materials	21
Public communication	25
Project website	26
Interactions with EU e-infrastructure projects and initiatives	28
CONCLUSION	31
GLOSSARY	32
REFERENCES	32
ANNEXES	33
Annex 1. List of relevant events organised or attended by OpenRiskNet members	33
Annex 2. Webinar reports	33
Annex 3. Booklet of the final OpenRisknet workshop	33
Annex 4. List of resources and training materials generated by the project	33
Annex 5. Google Analytics for OpenRiskNet websites	33
Annex 6. eInfraCentral Benchmarking Report (Feb 2019) on Service Catalogue Maturity for OpenRiskNet	33

SUMMARY

This report describes the dissemination and training activities undertaken by the OpenRiskNet partners in the second half of the project (Jun 2018 - Nov 2019) and it is a continuation of **Deliverable 3.4** that reported the dissemination and training activities up to month 18 (Dec 2016-May 2018). In this report we followed a similar structure, including details on the relevant activities developed within the project: organisation of webinars, workshops, training events and hackathons, participation at conferences and workshops, peer-reviewed publications, tutorials, public communication activities, as well as the interactions initiated with other EU infrastructures or projects to support uptake of the services and their sustainability.

The dissemination activities are also listed on the project website, especially on the two interlinked sections:

- **Events:** Webinars, Symposiums, Hackathons, Trainings, Conferences, Workshops, Exhibitions and Project meetings;
- **Resources & Training:** Webinar recordings, Tutorials, Presentations, Posters, Public communication, Reports and Peer-reviewed publications.

Important announcements and highlights from the projects were also posted in the **News** section of the project website and shared using other communication channels (social media, newsletters, etc.).

These sections and the structure of the website facilitated the collection, sharing and reporting of the project activities relevant to the training, dissemination and exploitation activities addressed in WP3 (Training, Support and Dissemination), across WPs and to the OpenRiskNet consortium in general as well as ensuring optimal dissemination to all stakeholder groups.

The report is aligned with the OpenRiskNet **Plan for the Exploitation and Dissemination of Results (PEDR)** (*available as an Annex to the second Periodic Report*) which was used as a basis for the dissemination activities and exploitation strategies utilised in the project.

INTRODUCTION

To foster the worldwide adoption of OpenRiskNet solutions, a wide range of dissemination and networking activities were planned and executed. The activities in the first half of the project were reported in **Deliverable 3.4** [1] and also in the first two versions of the Plan for the Exploitation and Dissemination of Results (PEDR), while in this document we are concentrating on different dissemination activities executed in the second half of the project (last 18 months). 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. Generally, the dissemination activities conducted had the following main objectives:

- Communicate to the broader community in order to generate interest in the OpenRiskNet e-infrastructure;
- 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 service developers in plugging additional services into the OpenRiskNet e-infrastructure;
- Develop close interactions with stakeholders in order to identify additional funding opportunities, further support its development and implementation into risk assessment activities.

These activities, focused on the main targeted audiences of the project, represented by its stakeholders including end users like academic and industrial researchers, risk assessors, etc. as well as by the service developers (tools developers, data managers, e-infrastructure providers or system administrators).

The current report specifically includes the organisation of webinars, workshops, training events and hackathons, participation in conferences and trade shows, publications, and communication activities, enhancement of the project website, use of external tools (e.g., [Zenodo](#), [OpenAIRE](#), [EOSC/eInfraCentral portals](#), [FigShare](#) or [TeSS](#) the Elixir's Training Portal) or social media (e.g., [Twitter](#), [LinkedIn](#)). The range of dissemination tools and approaches utilised during period 2 is shown in **Table 1**:

- **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/>
- **Social Media**
 - Twitter
 - LinkedIn
- **External tools for dissemination**
 - Zenodo
 - OpenAIRE
 - EOSC / eInfraCentral
 - FigShare
 - Elixir's TeSS
 - YouTube

These resources related to the Events, Library, Services and Case studies descriptions and catalogues were integrated into the **project website** and were interlinked in order to fully exploit all materials generated within the dissemination activities, link them to their applications and make them easily accessible by users. The concept and one representative example are included in **Figure 1**, showing the approach applied for the exploitation of the resources generated from webinars. This concept, first developed and implemented in OpenRiskNet, that applies to some extent to most of the dissemination activities conducted in the project, was also adopted with success by other infrastructure projects, like NanoCommons.

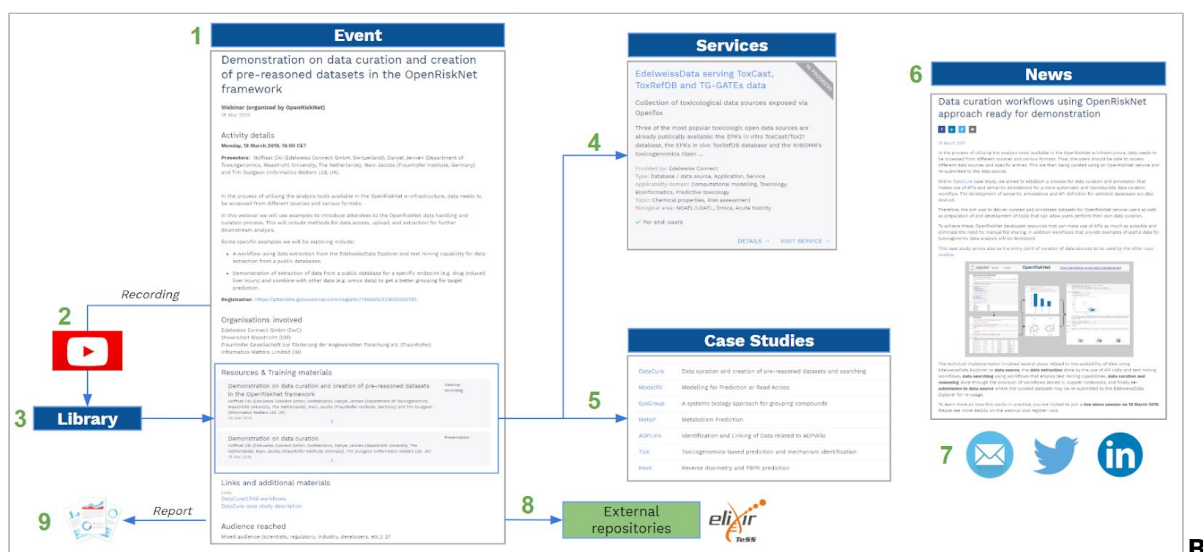
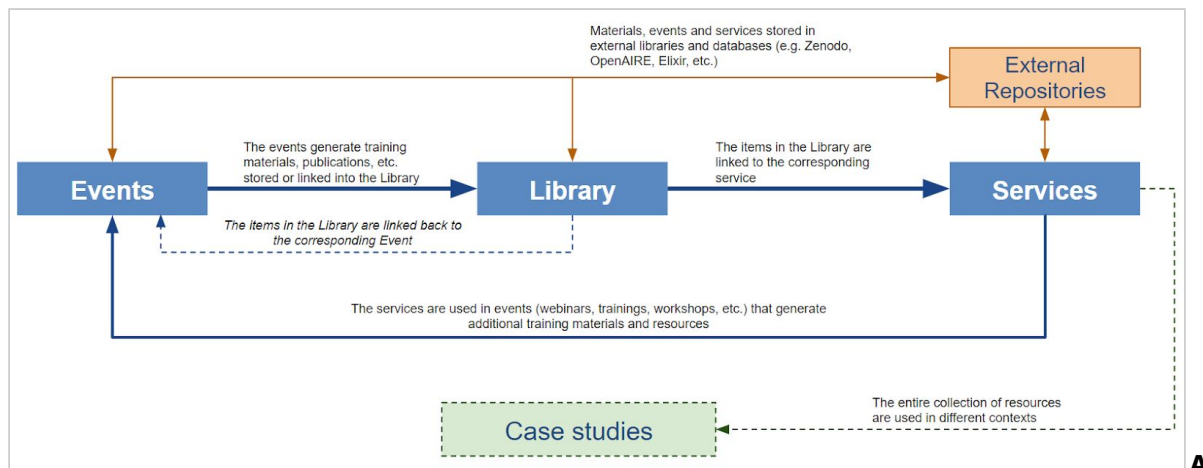


Figure 1. The concept developed in OpenRiskNet for collecting and interlinking the project resources (A) and one relevant example of resources generated, exploited and shared from the webinars (B)

Explanation to Figure 1.B - the Event (1), in this example a live webinar, was recorded and uploaded to YouTube (2), the recordings and all additional materials like slides were included in the project Library (3); these resources were also linked to the relevant services (4) and case studies (5), thus each service or case study description provides direct access to the training materials; The topic of the event was also included in News posts (6), including details on the development status or other achievements, and also advertising the event. Finally such materials were shared via Social Media (7), the events were listed in external repositories (8), and documented in an event report (9).

DISSEMINATION & TRAINING ACTIVITIES

Events

During the second part of the project (June 2018–November 2019), OpenRiskNet partners have been engaged in several online and F2F events (e.g., webinars, trainings, workshops, conferences) in order to present and demonstrate the achievements of the projects and its e-infrastructure, and to reach out to the relevant stakeholders (**Figure 2**). Activities were aimed mainly externally in order to interact with the community and receive feedback on OpenRiskNet’s current status and identify future opportunities. These events generated a rich source of materials (training materials, tutorials, presentations, etc.) that were collected in the project Library and further exploited to the benefit of the OpenRiskNet stakeholders.

Some relevant examples are described below, while the complete list of events organised or attended by OpenRiskNet members is included in **Annex 1**.

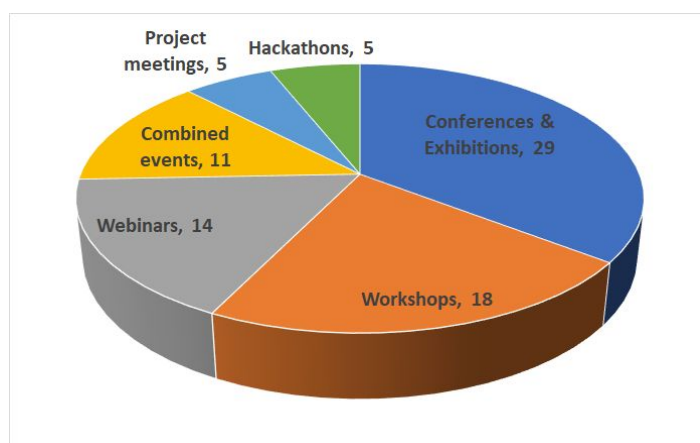


Figure 2. Number and categories of events organised, co-organised and attended by OpenRiskNet members

Organisation of webinars

With ten webinar sessions organised in 2019 and four introduction sessions in 2018 (see **Table 1** and **Figure 2**), OpenRiskNet undertook outreach to representatives from different sectors and areas like risk assessment, e-infrastructures, nanosafety, modelling, toxicology, AOPs or regulatory (**14 sessions** with **~250 logins**).

All materials produced during these sessions (video recordings, slides, additional resources) are available online (i.e., YouTube, see **Figure 3**)

but can also be accessed directly from the OpenRiskNet [Events page](#)¹, or from the [Library](#)



¹ <https://openrisknet.org/events/webinars>

[page](#)² by selecting the relevant category of training materials.

Table 1. List of webinars organised by OpenRiskNet, including a link to their description and all resources generated (recordings, slides)

Topic	Link to the description and date
Introduction sessions to the OpenRiskNet e-infrastructure	<ul style="list-style-type: none"> • 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)

The OpenRiskNet webinars series included live demonstrations of the e-infrastructure deployment and the risk assessment case studies. These case studies (see **Deliverable 1.3** [2] and **Deliverable 1.5**) aimed to demonstrate the OpenRiskNet infrastructure capabilities and to test different risk assessment scenarios. The case studies offered examples and prototypes for solutions provided to the predictive toxicology and risk assessment community and demonstrated the usage of the developed APIs and the interoperability

² <https://openrisknet.org/library/>

features to build integrated workflows. The case studies also demonstrate how OpenRiskNet offers customised approaches for the different stakeholder groups (e.g. researchers, risk assessors or 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). All these aspects were covered within the live demonstration sessions. The reports of the webinars organised in 2019 are included as **Annex 2**.















1	 Introduction to OpenRiskNet project Edelweiss Connect, Switzerland	8	 Identification and linking of data related to AOPWiki Edelweiss Connect, Switzerland
2	 Introduction to OpenRiskNet e-infrastructure Edelweiss Connect, Switzerland	9	 OpenRiskNet webinar: AOP Database Edelweiss Connect, Switzerland
3	 OpenRiskNet case studies and the implementation challenge Edelweiss Connect, Switzerland	10	 OpenRiskNet webinar: Semantic annotations Edelweiss Connect, Switzerland
4	 OpenRiskNet webinar: introduction, case studies and demo (Part 1) Edelweiss Connect, Switzerland	11	 OpenRiskNet Webinar: Use Nextflow for toxicogenomics-based prediction Edelweiss Connect, Switzerland
5	 OpenRiskNet webinar: demonstrations on services (Part 2) Edelweiss Connect, Switzerland	12	 ORN Webinar: Deploying Applications to an OpenRiskNet Virtual Environment Edelweiss Connect, Switzerland
6	 OpenRiskNet deployment Edelweiss Connect, Switzerland	13	 OpenRiskNet webinar: Approach on modelling for prediction or read across Edelweiss Connect, Switzerland
7	 Data curation demonstration Edelweiss Connect, Switzerland	14	 ORN Webinar: Connecting AOPs, knowledge and data with AOPLink workflows Edelweiss Connect, Switzerland

Figure 3. OpenRiskNet webinar recordings collection in YouTube³

Following the webinars, participants were asked to complete a feedback survey. Here are some examples of suggestions received and below some statistics on the participants profile (**Figure 4**):

- 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.

These suggestions were considered and implemented in the subsequent webinars and also included when the final workshop (*see the next section*) was designed.

³ <https://www.youtube.com/playlist?list=PLTxsS5QQK1ymTJPa2aTIGfUNLt-3M4I0>



Figure 4. Participants profile and feedback (webinars)

Organisation of workshops, trainings and hackathons

User-driven F2F events were organised or co-organised jointly with other EU projects. These included workshops and training sessions, e.g., Hands-on Workshop on Biokinetics Modelling⁴, Building risk assessment workflows with OpenRiskNet (hands-on workshop)⁵ and ontological annotation of datasets⁶ - sessions included in the OpenTox Conference October 2018, OpenRiskNet/NanoCommons ontology meeting December 2018⁷ and the Final OpenRiskNet Workshop⁸ organised on 23-24 October 2019 in Amsterdam, The Netherlands. The latter, as the main event of OpenRiskNet in the second period, is described in more detail below.

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

The event aimed to disseminate the achievements and implemented concepts of the project, make the stakeholders aware of the solutions developed and find the best options for the adoption of the services by other projects or organisations. The event offered the opportunity for the OpenRiskNet services users, developers and administrators as well as the members of related e-infrastructure communities like EOSC and NanoCommons to interact with OpenRiskNet developers, modellers and project managers. Strong focus was put on documenting and showcasing experiences from the community building efforts fostered by the associated partner programme and the implementation challenges, as well as on establishing and strengthening links to other projects and organising the transfer of the technology into further initiatives presented by both sides, consortium members and even more importantly associated partners.



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/>

The workshop was attended by **53 participants**, representing all OpenRiskNet stakeholders (scientific, industrial and regulatory communities). This ensured that all relevant and targeted groups that need to be aware of the project achievements have access to this information and are enabled to give feedback, and also be trained on the provided solutions (**Figure 5**).



⁴ <https://openrisknet.org/events/50/>

⁵ <https://openrisknet.org/events/51/>

⁶ <https://openrisknet.org/events/46/>

⁷ <https://openrisknet.org/events/45/>

⁸ <https://openrisknet.org/events/74/>

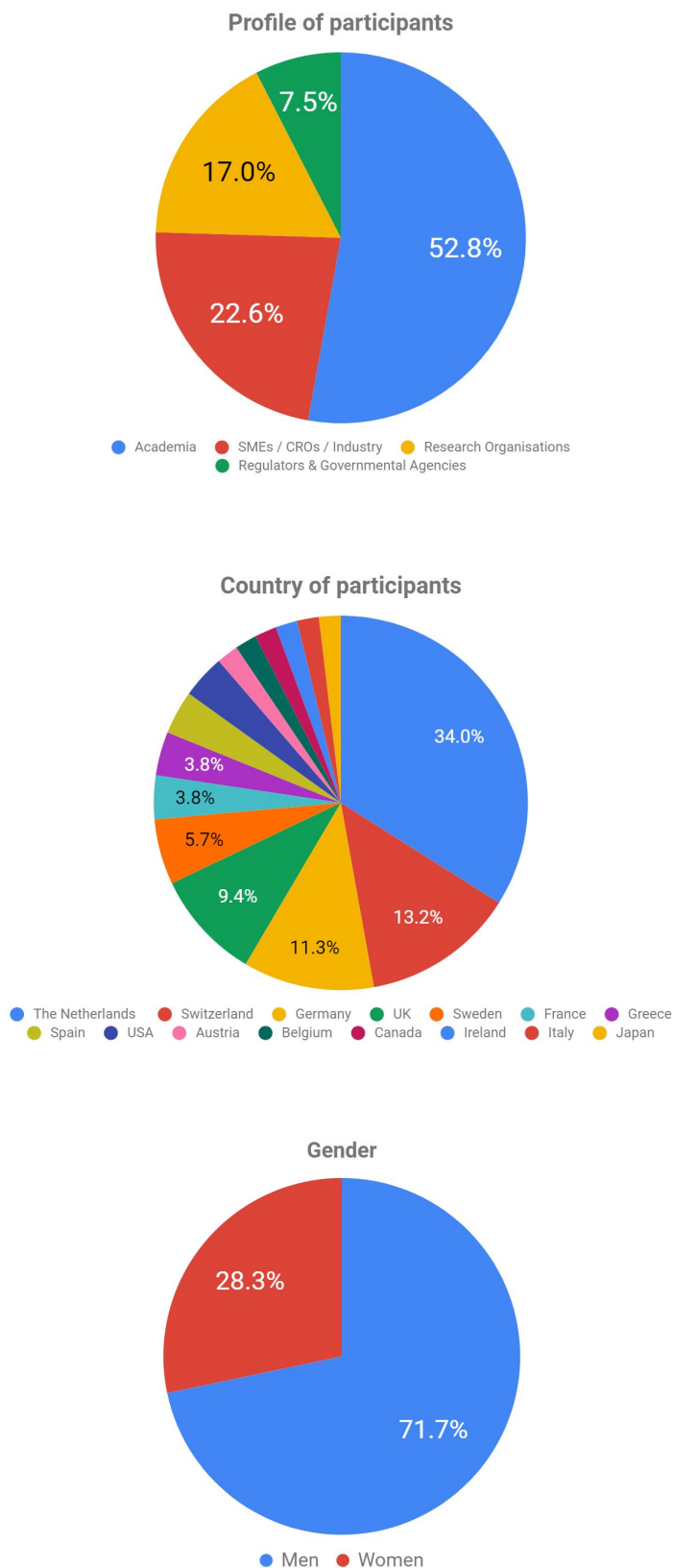


Figure 5. Participants profile at the OpenRiskNet final workshop

The first part of the 2-day event focused on the OpenRiskNet case studies, demonstrations, posters and hands-on training sessions, where the teams involved in the development and implementation presented and demonstrated the use of the services included in the OpenRiskNet e-infrastructure covering all aspects from setting up the infrastructure and virtual environments, deploying services to the use of specific services, combining them and their use in complex workflows to address specific risk assessment tasks. Presentations included:

- Case studies flash presentations
- Workflows: practical example of Jupyter notebooks use, Data curation example, workflow across multiple case studies
- Deploying Applications (addressed to developers, services providers and infrastructure administrators)
- Modelling exercise (built around the ModelRX case study, support of the DataCure) (addressed to end-users)
- Ontology and semantic annotations.
- For much of this time, participants self-selected which of the hands-on sessions to participate in, with 2 sessions running in parallel.



The second day focused on the outreach and sustainability aspects of the project. The associated partners and Implementation Challenges winners presented their achievements and the status of the integration of their services in the e-infrastructure, including:

- Strategy used to build confidence in PROSILICO's in silico methods for prediction of human clinical ADME/PK
- FAME 3: Predicting the Sites of Metabolism in Small Molecules for Phase 1 and Phase 2 Metabolic Enzymes and FAME 3 API in OpenRiskNet
- Using SPARQL to explore human protein data in neXtProt and beyond
- ToxicoGx: An R platform for integrated toxicogenomics data analysis
- US EPA AOP-DB: A database resource for the exploration of Adverse Outcome Pathways
- ToxPlanet: demo, information on API, discussion on use case scenarios

This session was concluded by a lecture and demonstrations on Diamond Light Source as the OpenRiskNet's first external Virtual Environment deployment, and the lessons learned from the associated partner programme.



Figure 6. Talks and poster presentations given at the OpenRiskNet final workshop

The final but very important topic of this event was related to the project sustainability measures, the support and maintenance of the infrastructure after the end of the project. Collaborations and links created with other communities were presented and discussed with representatives of other major pan-European infrastructures and policy makers like NanoCommons⁹ and EOSC (including here EOSC-hub, OpenAIRE or eInfraCentral).

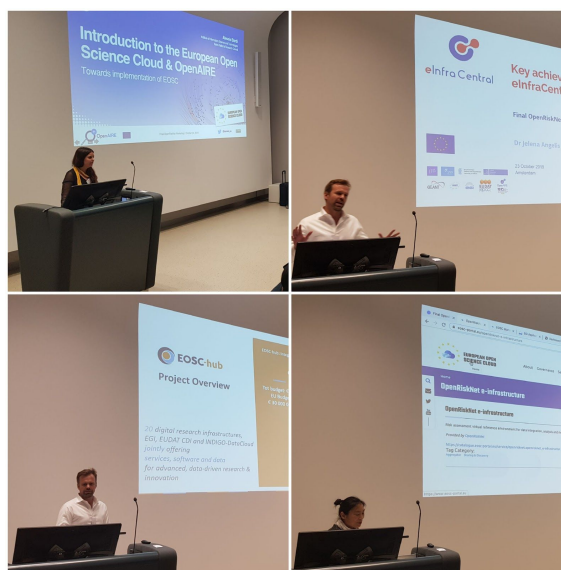


Figure 7. Talks given by the EOSC representatives at the OpenRiskNet final workshop

The adoption of OpenRisknet solutions by the NanoSafety community and NanoCommons infrastructure was shown, while the EOSC session included several lectures and demonstration:

- Introduction to the European Open Science Cloud (EOSC) and OpenAIRE: an EOSC

⁹ <https://www.nanocommons.eu/>

implementation project

- eInfraCentral: an EOSC implementation project
- EOSC-hub: an EOSC implementation project
- Technical demo of cloud and storage services in EOSC

The workshop concluded with a panel discussion on the lessons learned and next steps, funding opportunities and alignment with EOSC initiative, services marketplace and the EOSC early adopters calls.

The booklet of this event (including the complete description, agenda and abstracts - see **Annex 3**), all presentations and demonstration materials were made available on the event webpage¹⁰ and a workshop report was published online¹¹, distributed to Social Media channels and newsletters.

As an immediate follow-up to the event, a survey was distributed to the workshop participants in order to collect feedback regarding their profile (e.g. role in their organisations, level of experience, methods used and options used to access OpenRiskNet services) (**Figure 8**). On top, the participants were asked to evaluate the case studies, the sessions of the workshop and overall, the OpenRiskNet services, with responses presented in **Figure 9**.

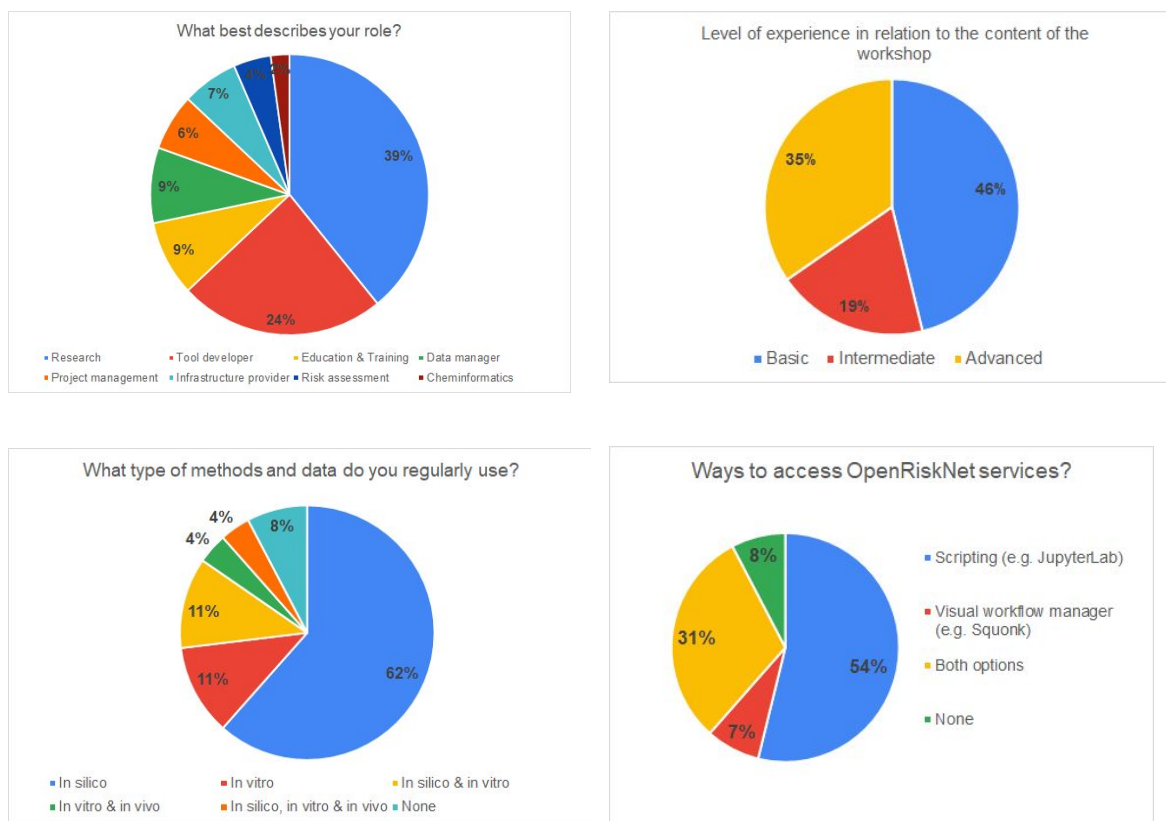


Figure 8. Participants feedback regarding their profile and the OpenRiskNet tools

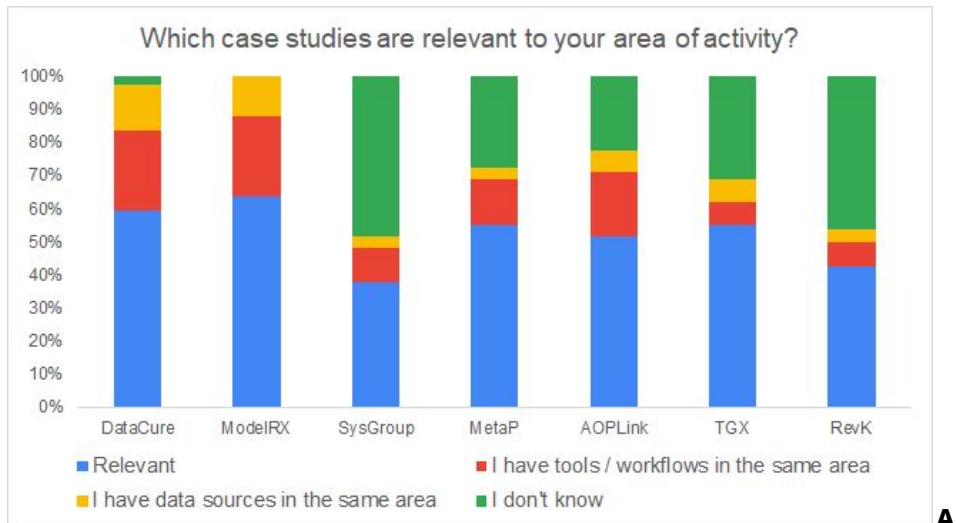
¹⁰ <https://openrisknet.org/events/74/>

¹¹ <https://openrisknet.org/news/29/>

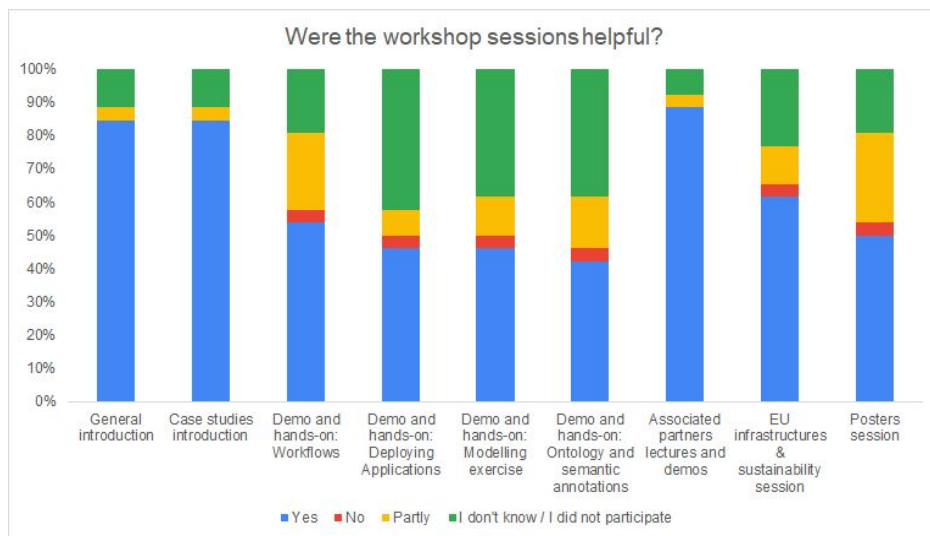
The profiles of the participants confirm observations made already in different outreach activities. OpenRiskNet is at the moment of most interest to users already having a background in development and/or utilisation of *in silico* methods. This includes researchers using such tools in their daily work but even more importantly, academic and commercial developers of services, which can run on the OpenRiskNet platform. However, with a fully functional infrastructure now, these service developers are empowered to create user-friendly applications for their customers who are typically experimental researchers, risk assessors and regulators. The validity of this approach - OpenRiskNet supporting service provider supporting end users - was shared by all participants (personal communication) and expressed in the statement of Reginald FitzGerald, Swiss Centre for Applied Human Toxicology: *“Overall, I was very impressed by the quality of the OpenRiskNet contributions, the workshop presentations and workshop organisation. In vitro/in silico toxicology is developing very rapidly, and the OpenRiskNet project exemplifies the collaborative work and communication which are essential for shaping the future.”*

With respect to the feedback on the sessions of the workshop, we can conclude that the training sessions fulfilled their purpose. All sessions were evaluated as useful or partly useful by a large majority of participants. Please note that the demo and hands-on sessions were run in parallel so that the *“I don’t now/I did not participate”* category are mainly the participants of the other training running in parallel. In our opinion, also the evaluation of the relevance of the case studies demonstrates the success of the presentations. The case studies, which were the subjects of the demo sessions and, in this way, described in more detail than in the flash presentations, were seen as very relevant, with ModelRX and DataCure reaching almost 100% approval and AOPLink being above 75% (sum of “Relevant”, “data source” and “tools/workflows”). All others except two have a good majority in favor. The reasons for participants to evaluate the two remaining case studies with *“I don’t know”* are that one (SysGroup) was not able to reach its full potential due to time limitations (see also **Deliverable D1.5**) and the complexity of biokinetics modelling (RevK) made it difficult for completely new users to follow in real-time.

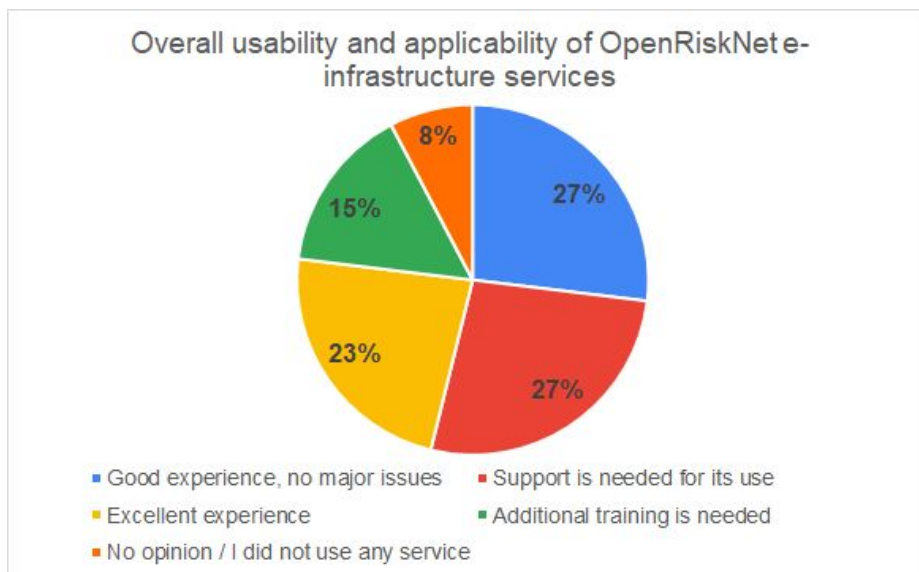
Additionally, recommendations and questions were received that refer especially to training and dissemination materials or support on the e-infrastructure implementation. To cover these aspects, the OpenRiskNet Library and Services Catalogue is continuously extended to contain and offer access to a rich source of materials regarding the use of the services, while additionally a direct contact is established by service providers with their users to provide tailored one-to-one support.



A



B



C

Figure 9. Participants feedback regarding case studies (A), different sessions (B) and overall OpenRiskNet services (C)

Participation at conferences and workshops

Similarly to the first part of the project, relevant events were attended by the OpenRiskNet members in order to promote the project achievements (>45 events attended in the last 18 months). The members of OpenRiskNet promoted the project by presenting posters, giving talks or being part of the exhibition booths. As mentioned above, the complete list of events is included in **Annex 1**, while the materials used for this events are available in the project Library. Here a selected list of major events where OpenRisknet was represented is provided:

- 54th Congress of the European Societies of Toxicology (EUROTOX), 2 – 5 Sep 2018 / Brussels, BE
- RDKit User group meeting, 19 - 20 Sep 2018 / Cambridge, UK
- UK QSAR meeting, 26 Sep 2018 / Oxford, UK
- 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

From these, the ToxExpo, where OpenRiskNet had a joint booth with other projects in a very exposed location of the exhibition hall (see photo in **Figure 10** below), and the ISMB/ECCB, where four interlinked posters were presented describing the general concepts and the case studies, had the most visibility.



Figure 10. SOT/ToxExpo 2019 booth shared between OpenRiskNet and other projects

Resources and training materials

Comprehensive resources and training materials were generated in order to support OpenRiskNet stakeholders in getting familiar with the services and tools available in the e-infrastructure (**Figures 11** and **12**). These were collected in the project Library and include tutorials and video demonstrations, publications (e.g. peer-review articles, presentations, posters) that aim to help users in their adoption of the OpenRiskNet concepts and implementations. The complete list of resources and training materials generated by the project is included in **Annex 4**.

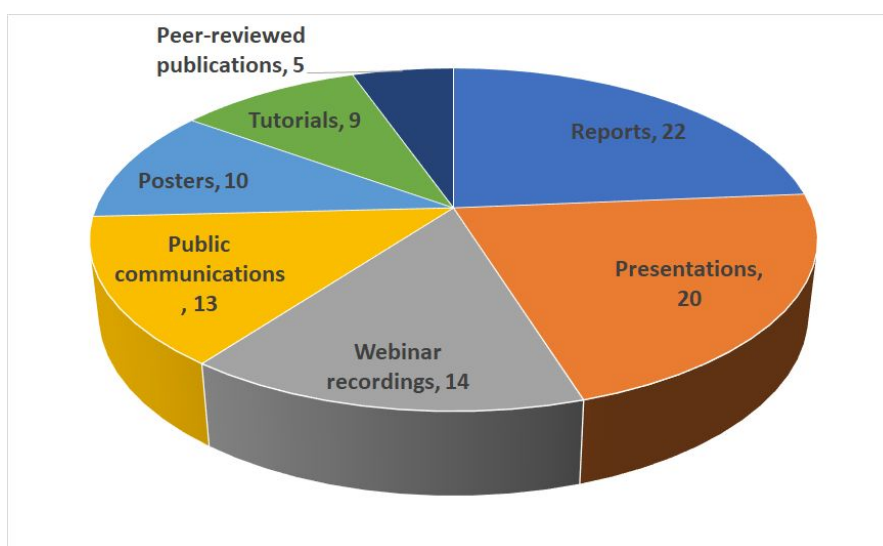


Figure 11. Resources & training materials available in the OpenRiskNet library

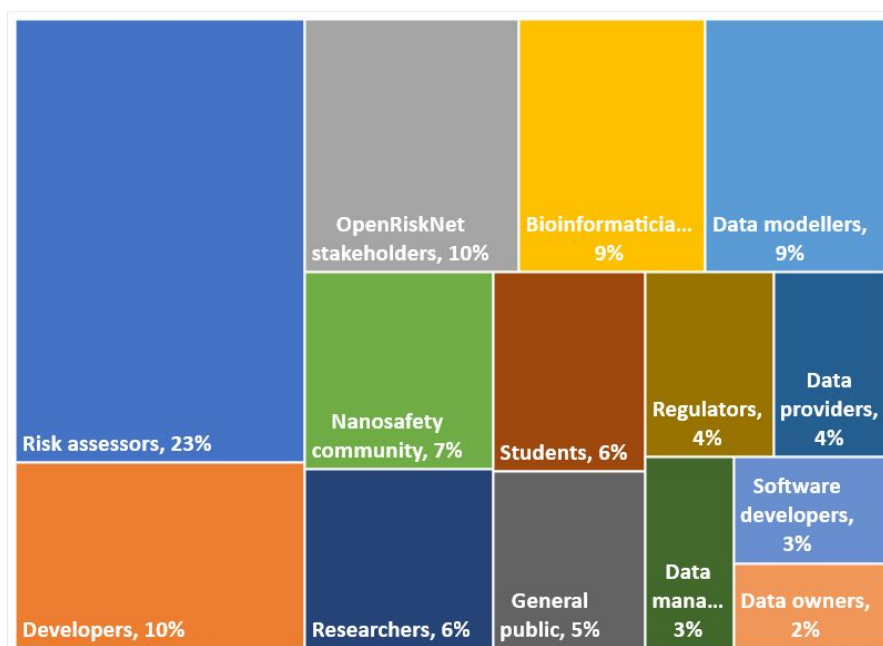


Figure 12. Distribution of resources to different target audiences

Five **open access peer-reviewed articles** were published over the period of the project based on, or using the OpenRiskNet concept and its e-infrastructure:

- Tsiros P, Bois FY, Dokoumetzidis A, Tsiliki G, Sarimveis H. Population pharmacokinetic reanalysis of a Diazepam PBPK model: a comparison of Stan and GNU MCSim. *J Pharmacokinet Pharmacodyn.* **2019**; 46: 173–192.
- Martens M, Verbruggen T, Nymark P, Grafström R, Burgoon LD, Aladjov H, et al. Introducing WikiPathways as a Data-Source to Support Adverse Outcome Pathways for Regulatory Risk Assessment of Chemicals and Nanomaterials. *Front Genet.* **2018**; 9: 661.
- Lampa S, Alvarsson J, Arvidsson Mc Shane S, Berg A, Ahlberg E, Spjuth O. Predicting Off-Target Binding Profiles With Confidence Using Conformal Prediction. *Front Pharmacol.* **2018**; 9: 1256.
- Lapins M, Arvidsson S, Lampa S, Berg A, Schaal W, Alvarsson J, et al. A confidence predictor for logD using conformal regression and a support-vector machine. *J Cheminform.* **2018**; 10: 17.
- Boudellioua I, Mahamad Razali RB, Kulmanov M, Hashish Y, Bajic VB, Goncalves-Serra E, et al. Semantic prioritization of novel causative genomic variants. *PLoS Comput Biol.* **2017**; 13: e1005500.

Additionally, a joint publication presenting the OpenRiskNet case studies implementation is planned and is based on the structure of **Deliverable 1.5**. In collaboration with the Horizon 2020 project PhenoMeNal¹², we have also collected experiences from working with workflow systems and containers, in a recent preprint: <https://peerj.com/preprints/27141/> that will be submitted to a journal during 2019. Also, we anticipate to present the results related to the MetaP case study of in a manuscript on tools integration.

The participation at conferences or other events generated additional publications, like **posters and presentations** (with the abstracts included in conference proceedings) (**Figure 13**).

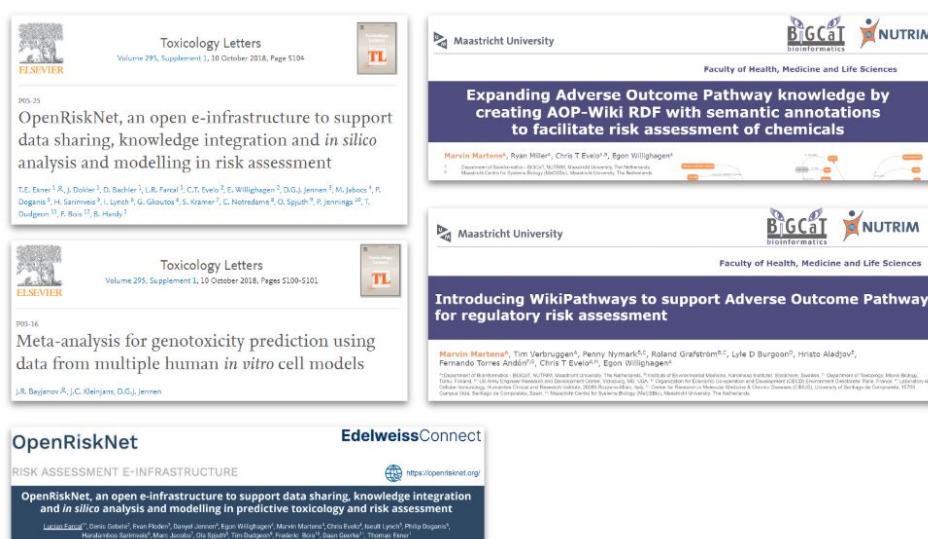


Figure 13. Selection of OpenRiskNet posters or publications in conference proceedings

¹² <http://phenomenal-h2020.eu/>

Besides these publications, the **public reports** represent an important documentation of the OpenRiskNet activities and were added to the Zenodo database (**Figure 14**) and also linked to the OpenAIRE portal and to the OpenRiskNet Library to achieve the highest possible visibility.

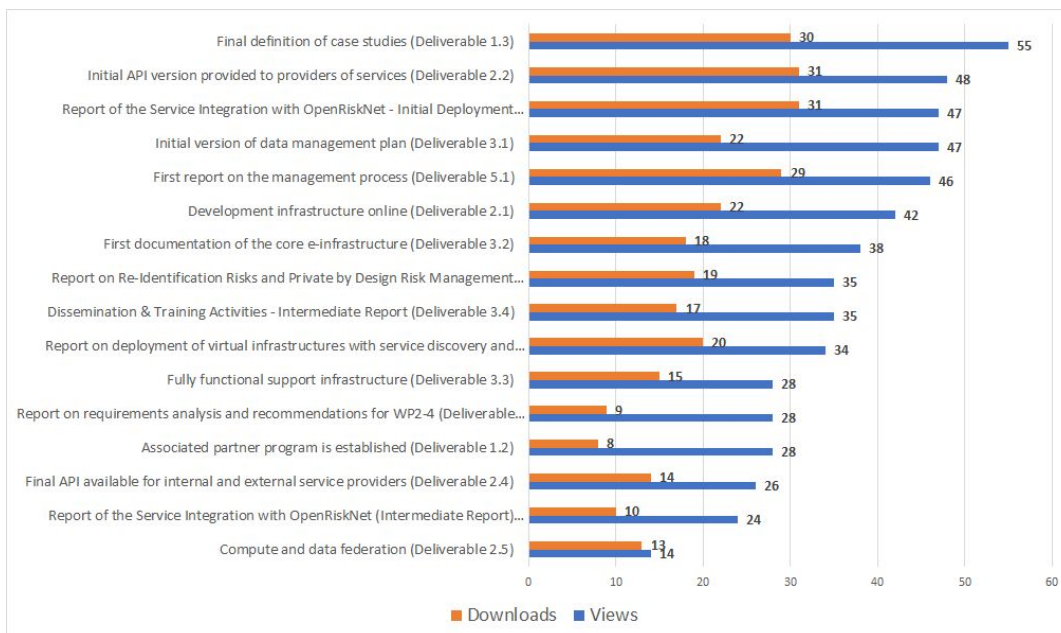


Figure 14. Number of downloads and views of OpenRiskNet deliverable reports in Zenodo (data from October 2019)

The effort on developing **tutorials and training materials** (see **Figure 15** for examples) continued also in the second half of the project, and these activities were aligned with the e-infrastructure deployment, case studies demonstration and services integration. On top of this, recorded webinars and workshops generated a rich collection of materials that can be used by OpenRiskNet users.

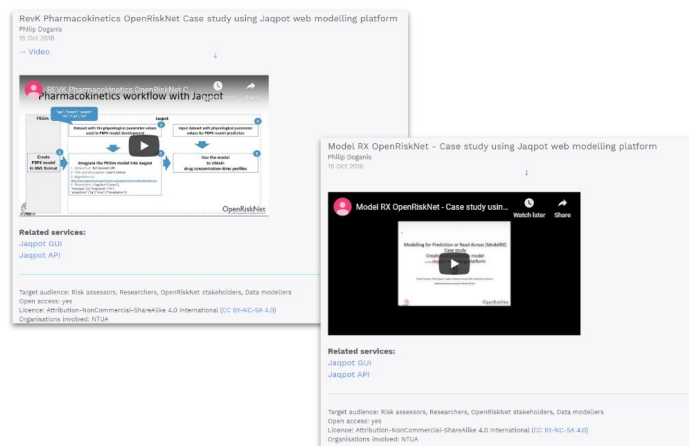


Figure 15. Examples of tutorials and training materials available from the OpenRiskNet library

To guide the stakeholders better to material most relevant to them, a user-driven approach was included into the project website, with sections dedicated to end-user and developers, respectively (the description of this concept and detailed information of the support infrastructure was included in **Deliverable 3.3** [3]). In brief, this tailoring includes:

- **Resources for end-users:** for scientists and researchers who would like to use the infrastructure for their predictive toxicology and risk assessment tasks;
- **Resources for developers:** for service developers, infrastructure providers or data managers who would like to integrate their databases and software tools into the OpenRiskNet infrastructure.

Public communication

Besides publications and participating in different events (as shown above), a major effort was also put on communicating the project developments using other communication channels like the News section of the project website (~30 items published in the last 18 months), external newsletters (NanoSafety Cluster) or social media (Twitter, YouTube and LinkedIn) (**Figure 15**).

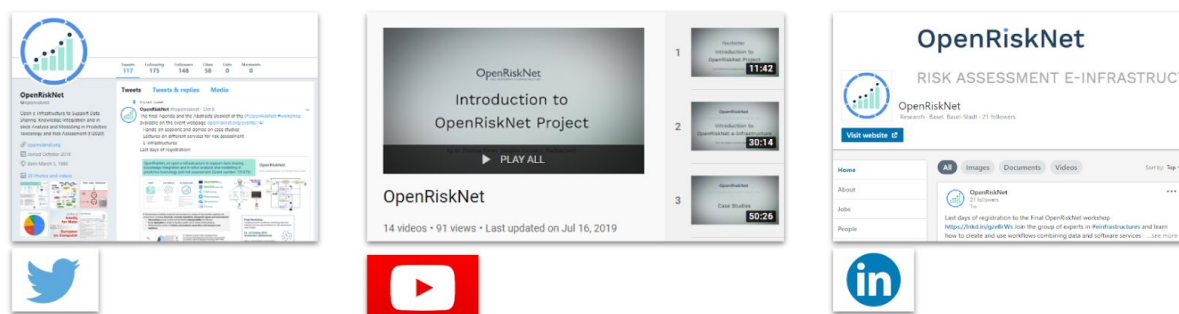


Figure 16. Main social media channels used by the OpenRiskNet consortium

The posts included highlights of new releases, announcements or articles focused on case studies and their demonstration (**Figure 17**). Additionally, different versions of project flyers, fact-sheets and one roll-up were created and used to advertise the project during events and other meetings.

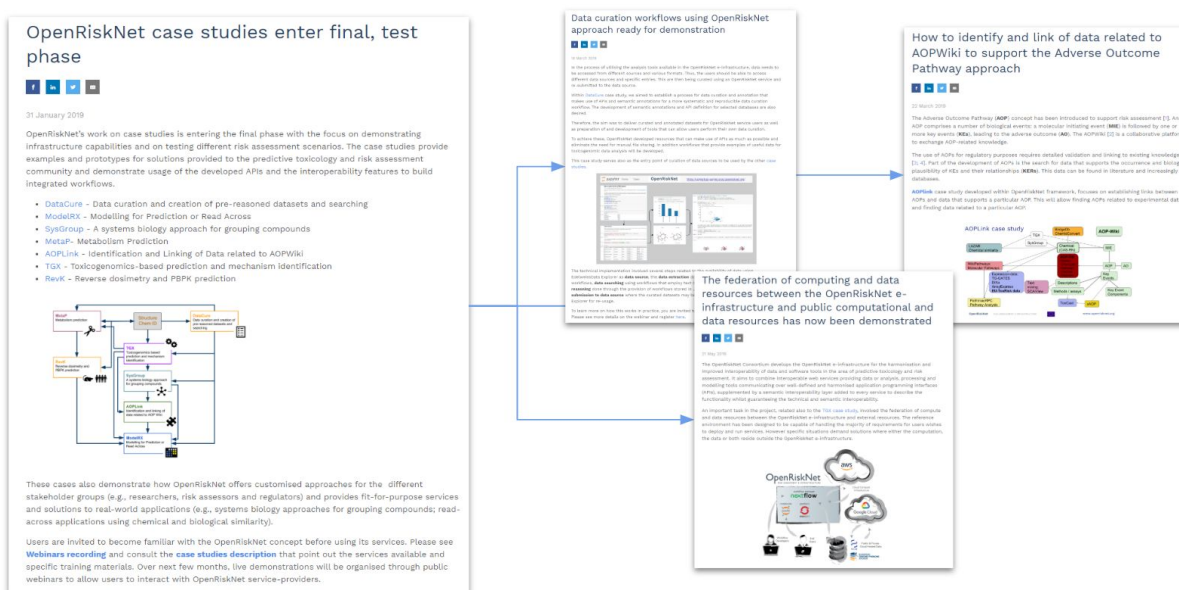


Figure 17. Series of News posts on the case studies and their demonstration sessions

Project website

The OpenRiskNet website was continuously developed and enhanced in order to enable presentation of project work and outputs to its stakeholders, the scientific community and to the general public. The website contains information on project objectives and partners, detailed information on the Associate Partner and Implementation Challenge Programmes and a list of dissemination activities (events, publications and other resources). On the technical development side, the website provides information on case studies and associated use cases. The features of the websites (e.g. the **catalogue of services, resources & training**, list of **events**, etc.) aim to support all project stakeholders in browsing and accessing the information of relevance to them, be that the available services and/or resources addressed to their specific user group (e.g. SMEs, regulators etc).

The screenshot shows the 'OpenRiskNet services' page. At the top right is a 'Submit a service' button. Below the title are four filter dropdown menus: 'Category', 'Application', 'End-users', and 'Targeted users', followed by 'Filter' and 'Reset' buttons. The main content area contains four service cards, each with a status tag in the top right corner: 'In Progress' (grey) or 'Integrated' (green).
 1. **EdelweissData serving ToxCast, ToxRefDB and TG-GATEs data** (In Progress): Collection of toxicological data sources exposed via OpenTox. Provided by: Edelweiss Connect. Type: Database / data source, Application, Service. Applicability domain: Computational modelling, Toxicology, Bioinformatics, Predictive toxicology. Topic: Chemical properties, Risk assessment. Biological area: NOAEL/LOAEL, Omics, Acute toxicity. Targeted users: For end-users.
 2. **Jaqpot GUI** (Integrated): Generate, store and share predictive statistical and machine learning models. Provided by: National Technical University of Athens. Type: Application, Visualisation tool, Analysis tool, Processing tool, Trained model, Model generation tool, Model, Data mining tool, Workflow tool. Applicability domain: Computational modelling, Predictive toxicology. Topic: Predictive modelling. Targeted users: For end-users.
 3. **Lazar Toxicity Predictions** (Integrated): Toxicity predictions. Provided by: In silico toxicology gmbh, Johannes Gutenberg University. Type: Application, Helper tool, Trained model, Model, Service. Applicability domain: Toxicology, Predictive toxicology. Topic: Chemical properties, Risk assessment, Structure-activity relationship (SAR / QSAR). Biological area: Acute toxicity, Blood brain barrier, Carcinogenicity, NOAEL/LOAEL, Mutagenicity. Targeted users: For developers, For end-users.
 4. **ToxicoDB** (In Progress): A database for curated toxicogenomic datasets. Provided by: University Health Network. Type: Database / data source, Application, Visualisation tool, Software. Applicability domain: Bioinformatics, Predictive toxicology. Topic: Predictive modelling, Information extraction. Biological area: Transcriptomics. Targeted users: For end-users, For developers.

Figure 18. OpenRiskNet catalogue listing all available service (only a subset is shown here)

For example, the e-infrastructure catalogue (see **Figure 18**) provides a detailed description of the available services (e.g. on the type, category, applicability domain and topic, targeted industry or targeted users, biological area covered, etc.). Categorisation provided as metadata to each service supports the filtering and selection of appropriate services by the users. The description includes the direct links to the service environment and/or to the API definition and also to all related support resources (service provider, contact, information on the licence, resources and training materials). Moreover, the catalogue features tags (green for fully integrated, grey for in progress, as shown in the top right corner of each service as presented in **Figure 18**) describing the different status of the integration into the OpenRiskNet VRE.



Figure 18. News and events section on the OpenRiskNet website

The section on the resources & training lists all available publications (e.g. peer-review articles, posters, oral presentations) and tutorials (including video materials). These resources are linked to the OpenRiskNet services in the e-infrastructure and also to the News & events section (see **Figure 19**). The latter lists all events in advance so that the project stakeholders know where they could meet and interact with OpenRiskNet members, and highlighted the events organised or co-organised by OpenRiskNet.


The Google Analytics report for the project's websites for the last 6 months are included in **Annex 5** (data retrieved 26 November 2019). This is split into the project's main website, representing the general interest of the stakeholders in the project and specific programs like the Implementation Challenge and the training offers, and the entry page for the reference instance (production site) showing the use of the virtual environment. Overall almost 2,100 users have visited the OpenRiskNet sites with more than 10,000 page views. Examples of specific pages with high traffic are:

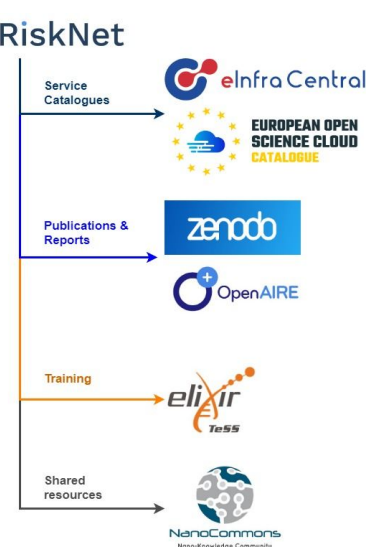
- | | |
|----------------------------------|-----------------|
| 1. Final workshop: | 1300 page views |
| 2. Services: | 557 page views |
| 3. Resources and training: | 466 page views |
| 4. Case studies: | 328 page views |
| 5. Associated partner programme: | 132 page views |

The start or landing page of the production site had 57 unique users and 182 page views. Both numbers are somewhat underestimating our user base. The single-sign-on system (SSO, see also **Deliverable D2.6**) of the reference instance (production site) registered 104 users, which is still a lower bound since it does not include users hosting their own virtual environment like Diamond Light Source and other tools do not require login into the SSO. This shows that the start page is just one way to access the reference infrastructure and that the users are accessing specific services specifically the Jupyter and Squonk notebooks services directly using the links provided in the service catalogue, the training material as well as the webinars. The project's Github is also widely used by developers and end-users of the tools and services.

Interactions with EU e-infrastructure projects and initiatives

The interactions and actions established with different e-infrastructure initiatives, towards disseminating, sustaining and exploiting the project were continuously developed (see details in the Plan for the Exploitation and Dissemination of Results). In summary, the interactions and collaborations established include:

- **EOSC and eInfraCentral:** dissemination of  OpenRiskNet platform and 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. Also, the ELIXIR's Training Portal was used. Finally, Thomas Exner was recently appointed to the ELIXIR industry advisory board;
- **EU NanoSafety Cluster and NanoCommons:** the nanosafety community represented one of the main beneficiaries of the OpenRiskNet services and continue to build on the OpenRiskNet platform and services;
- **EU-ToxRisk:** alignment with the major Horizon 2020 program working on a new approach and advanced risk assessment methods, “An integrated European ‘Flagship’ Programme Driving Mechanism-based Toxicity Testing and Risk Assessment for the 21st Century”;
- **PhenoMeNal** is a Horizon 2020 e-infra project that developed virtual research environments for metabolomics data analysis. We have built on the developments in PhenoMeNal and jointly expanded the work on using workflows within containers, which has resulted in a joint preprint publication (*to be submitted* <https://peerj.com/preprints/27141/>).



A major achievement was represented by the **inclusion of OpenRiskNet services into the European Open Science Cloud (EOSC) and eInfraCentral services catalogues**¹³ (Figure 20). This process included a permanent communication with the eInfraCentral / EOSC team, that was effective and useful as further recommendations were received, on both the registration process and also on the service descriptions. The initial registration process of OpenRiskNet as a service provider required the completion of certain steps for authorisation and evaluation of our application. Following this, the addition of new services to the catalogue was straightforward.

¹³ <https://einfracentral.eu/news/openrisknet-joined-eosc-catalogue>



Figure 20. OpenRiskNet e-infrastructure is accessible via the EOSC service catalogue enhancing visibility to users

The existing template provided by eInfraCentral, included a set of instructions and recommendations that were used in this process. As part of these interactions, a **“Benchmarking Report on Service Catalogue Maturity for OpenRiskNet”** was received, including an assessment round for the eInfraCentral/EOSC Catalogue maturity, with the sole purpose of improving our “service readiness” (see **Annex 6**). This report presented the results of a qualitative benchmarking analysis based on the OpenRiskNet public catalogue at OpenRiskNet website and the registrations at the eInfraCentral/EOSC Catalogue. General recommendations to improve the catalogue and related processes were provided along with a comparison to other service and resource providers. These recommendations were considered and implemented in a second iteration that led to an enhancement of the presence of the OpenRiskNet e-infrastructure in the EOSC Catalogue.

These interactions with the EOSC community were complemented by participating in different events, in both directions. Members of OpenRiskNet attended three EOSC related events (with posters and an introduction to OpenRiskNet):

- EOSC-hub Week, 10 – 12 Apr 2019 / Prague, CZ (**Figure 20**);
- EGI Workshop: Design your e-Infrastructure, 9 May 2019 / Amsterdam, NL;
- EC workshop “Building EOSC through the H2020 projects current status and future directions”, 9-10 Sep 2019 / Brussels, BE.



Figure 20. Presentation of OpenRiskNet at the EOSC-hub Week, 10-12 Apr 2019 (Prague, CZ)

Similarly, members of EOSC joined the final OpenRiskNet workshop and presented their projects in a dedicated session (*see the Events section above*). It is planned to continue and strengthen this interaction by the OpenRiskNet consortium and associated partners by becoming early adopters of EOSC-hub (an application to the early-adopter programme has been filed in October 2019 and is currently under evaluation).

CONCLUSION

During the last eighteen months (June 2018 - November 2019), OpenRiskNet partners intensified their efforts on dissemination and training activities, with the aim to increase the awareness on the e-infrastructure developed in the first part of the project, and to provide information and support on the OpenRiskNet services to potential users. The OpenRiskNet consortium supported and/or was involved in the organisation of a range of different events, targeting all categories of stakeholders that were reached out to during face-to-face or online events.

Over the whole duration of the project, OpenRiskNet members were involved in >80 events (>60 in the last 18 months), from which 22 were organised by OpenRiskNet (17 in the last 18 months) and 8 co-organised with other EU projects or organisations (6 in the last 18 months). OpenRiskNet was a participant / presenter (oral, poster, pop-up banner etc.) in the other 50 (37 in the last 18 months).

A rich collection of training materials and other support materials were generated (peer-reviewed publications, written or video tutorials and webinar recordings, reports, posters and public communication articles). All of these materials are easily accessible from the OpenRiskNet website and are logically linked to the relevant services, case studies or events.

An important activity was represented by the interactions established with the other EU e-infrastructures initiatives (EOSC community, including EOSC support projects, eInfraCentral, OpenAIRE, as well as ELIXIR and EU Nanosafety Cluster/NanoCommons communities). A major achievement is represented by the inclusion of OpenRiskNet services in the European Open Science Cloud (EOSC) catalogue of services and the even more intense integration of OpenRiskNet solutions into the EOSC marketplace is envisioned by participating in the early-adopter programme of EOSC-hub (the OpenRiskNet team submitted a proposal for the recent call, and is awaiting the outcome currently).

All these (openly accessible) resources offered to the scientific community as well as the networking activities of the project members increased the visibility of the risk assessment group/services within the larger EU e-infrastructure community and established the premise for future joint activities and developments aligned with the international initiatives in this area. These efforts will be sustained and possibly even intensified to continuously increase the user base, collaborate with global and neighboring infrastructures and, in this way, achieve long-term sustainability including also more and more commercial aspects (see the Sustainability Plan submitted as part of the second Periodic Report and PEDR).

GLOSSARY

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

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

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2. Jennings P, Exner T, Farcas L, Oki N, Sarimveis H, Doganis P, et al. Final definition of case studies (Deliverable 1.3). 2018. doi:10.5281/zenodo.1479127
3. Spjuth O, Farcas L, Lynch I, Dudgeon T, Exner T. Fully functional support infrastructure (Deliverable 3.3). 2019. doi:10.5281/zenodo.2558122

ANNEXES

Annex 1. List of relevant events organised or attended by OpenRiskNet members

Annex 2. Webinar reports

Annex 3. Booklet of the final OpenRisknet workshop

Annex 4. List of resources and training materials generated by the project

Annex 5. Google Analytics for OpenRiskNet websites

Annex 6. eInfraCentral Benchmarking Report (Feb 2019) on Service Catalogue Maturity for OpenRiskNet

Organiser	Co-organiser	Event name	Start date	End date	Location - city	Location - country	Categories	Website
√		Kick-off meeting of OpenRiskNet project	2016-12-15	2016-12-16	Basel	Switzerland	Project meeting	
√		First OpenRiskNet API workshop	2017-01-16	2017-01-17	Mainz	Germany	Workshop	
		Bioinformatics for Young inTernational researchers Expo (byteMAL)	2017-06-23		Maastricht	Netherlands	Conference	http://www.bytemal.org/
		OpenTox USA	2017-07-12	2017-07-13	Durham, NC	United States of America	Conference	http://www.opentox.net/events/opentox-usa-2017
		Open Science Fair (OSFair)	2017-09-06	2017-09-08	Athens	Greece	Conference	http://www.opensciencefair.eu/
	√	Nexflow: Reproducible in silico Genomics	2017-09-14	2017-09-15	Barcelona	Spain	Workshop	http://www.crg.eu/en/event/coursescrg-nextflow-reproducible-silico-genomics
		Big Data Training School for Life Sciences	2017-09-18	2017-09-22	Uppsala	Sweden	Training	https://www.embnet.org/wp/2017/07/03/big-data-training-school-life-sciences-18-22-september-2017-uppsala-sweden/
		RDKit UG	2017-09-20	2017-09-21	Berlin	Germany	Hackathon, Training	https://www.eventbrite.com/e/6th-rdkit-ugm-2017-tickets-32526309066
√		OpenRiskNet Developer Workshop	2017-09-25	2017-09-26	Uppsala	Sweden	Hackathon	https://pharmb.io/blog/orn-workshop-2017/
		2nd international de.NBI symposium "The Future Development of Bioinformatics Germany and Europe"	2017-10-23		Bielefeld	Germany	Symposium	http://www.denbi.de/symposium2017
√		1st annual meeting of OpenRiskNet consortium	2017-11-20	2017-11-21	Basel	Switzerland	Project meeting	
√		OpenRiskNet training	2017-11-21		Basel	Switzerland	Hackathon, Training	http://www.opentox.net/events/opentox-euro-2017/training-and-hackathon
		Openshift Commons meeting	2018-01-31		London	United Kingdom	Conference	
	√	OpenTox EURO	2017-11-22	2017-11-23	Basel	Switzerland	Conference	http://www.opentox.net/events/opentox-euro-2017
		SOT 57th Annual Meeting and ToxExpo	2018-03-11	2018-03-15	San Antonio	United States of America	Conference, Exhibition	http://www.toxicology.org/events/am/am2018/
		ICCA-LRI workshop 2018	2018-06-20	2018-06-21	Ottawa	Canada	Workshop	https://sites.google.com/site/iccalriworkshop2018/icca-lri-workshop-2018

Organiser	Co-organiser	Event name	Start date	End date	Location - city	Location - country	Categories	Website
		Nano Korea	2018-07-10	2018-07-13	Kintex	South Korea	Conference	http://sympo.nanokorea.or.kr/2018/eng/main/
		54th Congress of the European Societies of Toxicology (EUROTOX)	2018-09-02	2018-09-05	Brussels	Belgium	Conference, Exhibition	http://eventclass.org/contxt_eurotox2018/online-program
		European Conference on Computational Biology (ECCB)	2018-09-08	2018-09-12	Athens	Greece	Conference	http://eccb18.org/programme/
		3rd NanoSafety Forum for Young Scientists	2018-09-10	2018-09-12	Valletta	Malta	Conference	https://www.nanosafetycluster.eu/nsc-meetings/3rd-nanosafety-forum-for-young-scientists-malta-2018.html
		7th Annual Meeting of the ASCCT	2018-09-10	2018-09-11	Bethesda	United States of America	Conference	https://www.asccto.org/annualmeeting
		3rd Exchange of Experience Workshop on "Effective Use of Preparatory Phase Funding"	2018-09-12		Vienna	Austria	Workshop	https://www.esfri.eu/esfri-eeo-workshops/3rd-exchange-experience-workshop-eeo
		22nd European Symposium on Quantitative Structure-Activity Relationships (EuroQSAR)	2018-09-16	2018-09-20	Thessaloniki	Greece	Conference	http://www.euroqsar2018.org/
		SETAC Asia-Pacific Conference	2018-09-16	2018-09-18	Daegu	South Korea	Conference	http://www.setac-ap2018.org/
		RDKit UGM	2018-09-19	2018-09-21	Cambridge	United Kingdom	Hackathon, Workshop	https://www.eventbrite.com/e/7th-rdkit-ugm-2018-tickets-44883066460
		9th International Conference on Nanotoxicology (NanoTox)	2018-09-20	2018-09-21	Neuss	Germany	Conference	http://nanotox2018.org/
		21st European Congress on Alternatives to Animal Testing and 18th Annual Congress of EUSAAT	2018-09-23	2018-09-26	Linz	Austria	Conference	https://www.eusaat-congress.eu/
√		Introducing the OpenRiskNet e-infrastructure and demonstration	2018-09-24				Webinar	https://openrisknet.org/news/14/
		UK QSAR	2018-09-26		Oxford	United Kingdom	Workshop	http://ukqsar.org/index.php/2018/05/11/ukqsar-autumn-2018-date-notification/
√		Introducing the OpenRiskNet e-infrastructure to US Nano WG	2018-09-27				Webinar	https://openrisknet.org/news/14/
		French Society of Toxicology meeting	2018-10-01	2018-10-02	Paris	France	Conference	
		EU-ToxRisk TempOSeq analysis workshop	2018-10-04	2018-10-05	Leiden	Netherlands	Workshop	

Organiser	Co-organiser	Event name	Start date	End date	Location - city	Location - country	Categories	Website
√		OpenRiskNet e-infrastructure demonstration session	2018-10-04				Webinar	
		WikiPathways Summit	2018-10-08	2018-10-10	San Francisco	United States of America	Workshop	https://gladstone.org/WP18Summit
	√	1st NanoCommons Hackathon on "Ontological Annotation of Datasets"	2018-10-09		Athens	Greece	Hackathon	https://www.nanocommons.eu/1st-nanocommons-hackathon-ontological-annotations-of-datasets/
√		Hands-on Workshop on Biokinetics Modelling	2018-10-10		Athens	Greece	Workshop	http://www.opentox.net/events/opentox-euro-2018/program
	√	OpenTox EURO	2018-10-10	2018-10-11	Athens	Greece	Conference	http://www.opentox.net/events/opentox-euro-2018
√		Building risk assessment workflows with OpenRiskNet - Hands-on Workshop	2018-10-11		Athens	Greece	Workshop	http://www.opentox.net/events/opentox-euro-2018/s6
		US-EU Nano meeting	2018-10-11	2018-10-12	Washington DC	United States of America	Workshop	https://us-eu.org/2018-u-s-eu-workshop/
		20th International Congress on In Vitro Toxicology (ESTIV)	2018-10-15	2018-10-18	Berlin	Germany	Conference	https://www.estiv2018.com/
		InnovationWell Interaction Meeting	2018-10-18		Philadelphia	United States of America	Workshop	http://www.innovationwell.net/events/2018-philadelphia
		InnovationWell Interaction Meeting	2018-10-22		Boston	United States of America	Workshop	http://www.innovationwell.net/events/2018-boston-october
√		Introducing the OpenRiskNet e-infrastructure	2018-10-30				Webinar	
		American College of Toxicology Annual Meeting (ACT)	2018-11-04	2018-11-07	West Palm Beach	United States of America	Conference	https://www.dremed.com/medical-trade-shows/?p=6583
		ELIXIR's BioHackathon	2018-11-12	2018-11-16	Seine-Port	France	Hackathon	https://www.elixir-europe.org/events/biohackathon-2018-paris
		Nextflow: Reproducible in-silico genomics	2018-11-22	2018-11-23	Barcelona	Spain	Workshop	http://www.crg.eu/en/event/coursescrg-nextflow-reproducible-silico-genomics-0

Organiser	Co-organiser	Event name	Start date	End date	Location - city	Location - country	Categories	Website
		SST Annual Meeting 2018	2018-11-29	2018-11-30	Basel	Switzerland	Conference	http://www.swisstox.ch/swisstox-en/aktuelles/meldungen/62_sst_annual_meeting_2018.php
		11th International SWAT4HCLS Conference	2018-12-03	2018-12-06	Antwerp	Belgium	Conference	http://www.swat4ls.org/workshops/antwerp2018/
√		2nd annual meeting of OpenRiskNet consortium	2018-12-12	2018-12-13	Brussels	Belgium	Project meeting	https://openrisknet.org/events/44/
	√	OpenRiskNet/NanoCommons ontology meeting	2018-12-13	2018-12-14	Brussels	Belgium	Hackathon, Workshop	
		Openshift Commons meeting	2019-01-30		London	United Kingdom	Conference	https://commons.openshift.org/gatherings/London_2019.html
√		Learn how to deploy the OpenRiskNet virtual research environment	2019-02-25				Webinar	
		OpenTox Asia 2019	2019-03-01	2019-03-03	Hyderabad	India	Conference, Workshop	http://www.opentox.net/events/opentox-asia-2019
		SOT 58th Annual Meeting and ToxExpo	2019-03-11	2019-03-14	Baltimore	United States of America	Conference, Exhibition	https://www.toxicology.org/events/am/AM2019/
√		Demonstration on data curation and creation of pre-reasoned datasets in the OpenRiskNet framework	2019-03-18				Webinar	
√		Identification and linking of data related to AOPWiki (an OpenRiskNet case study)	2019-03-26				Webinar	
		UKQSAR Spring 2019	2019-04-04		Cambridge	United Kingdom	Conference	http://ukqsar.org/index.php/2019/01/10/ukqsar-spring-2019-cambridge/
	√	AOP-DB: The Adverse Outcome Pathway Database	2019-04-08				Webinar	
		EOSC-hub Week 2019	2019-04-10	2019-04-12	Prague	Czechia	Conference	https://www.eosc-hub.eu/events/eosc-hub-week-2019
		EGI Workshop: Design your e-Infrastructure	2019-05-09		Amsterdam	Netherlands	Workshop	https://indico.egi.eu/indico/event/4434/
√		How to describe OpenRiskNet services and their functionality by semantic annotation	2019-05-13				Webinar	

Organiser	Co-organiser	Event name	Start date	End date	Location - city	Location - country	Categories	Website
√		Use of Nextflow tool for toxicogenomics-based prediction and mechanism identification in OpenRiskNet e-infrastructure	2019-05-27				Webinar	
√		Demonstration on OpenRiskNet approach on modelling for prediction or read across (ModelRX case study)	2019-06-11				Webinar	
	√	Combining neXtProt and WikiPathways strengths using SPARQL federated queries	2019-06-12				Webinar	
		EuroNanoForum 2019	2019-06-12	2019-06-14	Bucharest	Romania	Conference, Exhibition	https://www.euronanoforum2019.eu/
		EAGSMT meeting	2019-06-19	2019-06-21	Paris	France	Conference	
√		Deploying Applications to an OpenRiskNet Virtual Environment	2019-06-24				Webinar	
		34th International Exhibition for Fine and Speciality Chemicals (Chemspeceurope 2019)	2019-06-26	2019-06-27	Basel	Switzerland	Conference, Exhibition	https://www.chemspeceurope.com/2019/english/
		Joint workshop NanoCommons - NanoSolveIT - RiskGONE	2019-07-04		Limassol	Cyprus	Workshop	
√		Connecting Adverse Outcome Pathways, knowledge and data with AOPLink workflows	2019-07-15				Webinar	
		ISMB/ECCB 2019 - International Conference on Intelligent Systems for Molecular Biology & European Conference on Computational Biology	2019-07-21	2019-07-25	Basel	Switzerland	Conference	https://www.iscb.org/ismbecb2019
		Building EOCS through the H2020 projects current status and future directions	2019-09-09	2019-09-10	Brussels	Belgium	Workshop	
		Rancher Rodeo	2019-09-25		Bristol	United Kingdom	Training, Workshop	https://rancher.com/events/rodeos/2019-09-25-rodeo-bristol/
		UKQSAR Autumn Meeting	2019-09-26		Nottingham	United Kingdom	Workshop	http://ukqsar.org/index.php/2019/07/26/ukqsar-autumn-meeting-26th-september-2019-sygnature-nottingham/
		e-Resources to Revolutionise Toxicology: Linking Data to Decisions	2019-10-07	2019-10-11	Leiden	Netherlands	Workshop	https://www.lorentzcenter.nl/ic/web/2019/1134/info.php3?wsid=1134&venue=Snellius

Organiser	Co-organiser	Event name	Start date	End date	Location - city	Location - country	Categories	Website
		RedHat Forum	2019-10-15		London	United Kingdom	Symposium, Training, Workshop	https://events.redhat.com/profile/form/index.cfm?PKformID=0x66425abcd
		Rancher Rodeo	2019-10-17		London	United Kingdom	Training, Workshop	https://rancher.com/events/rodeos/2019-10-17-rodeo-london/
√		3rd (final) annual meeting of OpenRiskNet consortium	2019-10-22		Amsterdam	Netherlands	Project meeting	
√		Final OpenRiskNet Workshop: Creating powerful workflows combining data and software services demonstrated on risk assessment case studies	2019-10-23	2019-10-24	Amsterdam	Netherlands	Workshop	
		OpenTox Euro 2019	2019-10-29	2019-10-31	Basel	Switzerland	Conference, Workshop	https://opentox.net/events/opentox-euro-2019
		EOSC-Life Hackathon	2019-11-14	2019-11-15	Berlin	Germany	Hackathon	http://www.eosc-life.eu/news/hackathon/
	√	OpenRiskNet final review meeting	2020-01-28		Luxembourg	Luxembourg	Project meeting	

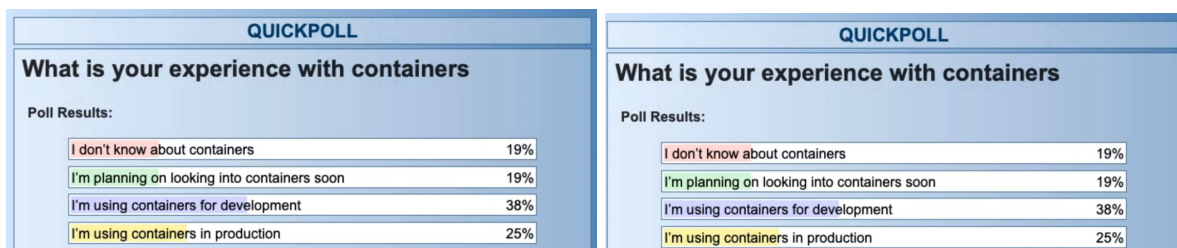
Webinar Report

Learn how to deploy the OpenRiskNet virtual research environment

Date	2019-02-25
Presenters	Alan Christie and Tim Dudgeon (Informatics Matters Ltd, UK)
Website	https://openrisknet.org/events/57/
Webinar recording	https://youtu.be/qOiOC09XRig
Slides	https://openrisknet.org/library/
Registrants	35
Attendees	23

The webinar included an introduction to the OpenRiskNet "OKD Orchestrator", a virtual environment (VE) deployment utility that simplifies the installation of the latest version of the OpenShift OKD container runtime. The main features of the orchestrator were shown together with installation process of the built-in example topologies to AWS EC2 and bare-metal (an OpenStack cluster in the SNIC Science Cloud (SSC)). The configuration file that controls the runtime topology allowing to create own installations were also explored.

Polls during the webinar

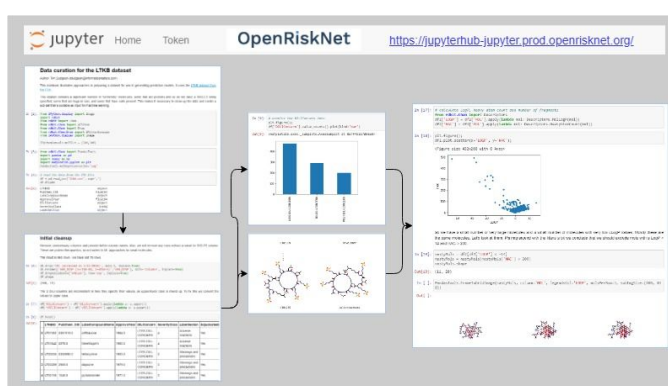


Webinar Report

Demonstration on data curation and creation of pre-reasoned datasets in the OpenRiskNet framework

Date	2019-03-18
Presenters	Noffisat Oki (Edelweiss Connect GmbH, Switzerland), Danyel Jennen (Department of Toxicogenomics, Maastricht University, The Netherlands), Marc Jacobs (Fraunhofer Institute, Germany) and Tim Dudgeon (Informatics Matters Ltd, UK)
Website	https://openrisknet.org/events/58/
Webinar recording	https://www.youtube.com/watch?v=KAXuViUqzY8
Slides	https://openrisknet.org/library/
Registrants	42
Attendees	27

In this webinar several examples on the OpenRiskNet data handling and curation process were demonstrated. This included methods for data access, upload, and extraction for further downstream analysis. Some specific examples explored includes a workflow using data extraction from the EdelweissData Explorer and text mining capability for data extraction from a public database, and demonstration of extraction of data from a public database for a specific endpoint (e.g. drug induced liver injury) and combine with other data (e.g. omics data) to get a better grouping for target prediction.¹



¹ <https://openrisknet.org/news/21/>

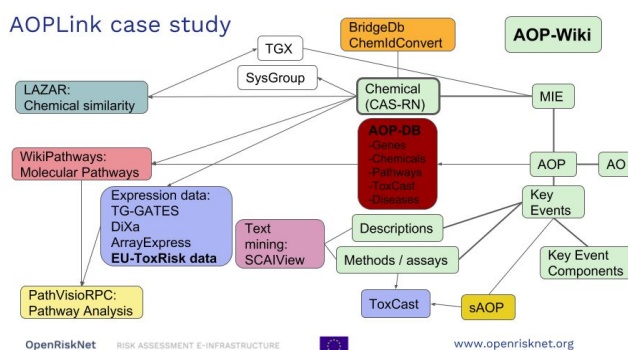
Webinar Report

Identification and linking of data related to AOPWiki (an OpenRiskNet case study)

Date	2019-03-26
Presenters	Marvin Martens and Egon Willighagen (Department of Bioinformatics, Maastricht University, The Netherlands), Thomas Exner (Edelweiss Connect GmbH, Switzerland)
Website	https://openrisknet.org/events/59/
Webinar recording	https://youtu.be/uS77xjhyo1A
Slides	https://openrisknet.org/library/
Registrants	26
Attendees	21

The webinar provided an introduction to the OpenRiskNet project and its case studies that are used to test and evaluate methods, workflows, and solutions for the predictive toxicology and risk assessment community.

One of these case studies is AOPLink, managed by Maastricht University, which aims for the validation and linking of existing knowledge to support Adverse Outcome Pathways (AOPs). The case study involves the establishment of links between AOPs and experimental data, chemical databases, and the molecular pathway database WikiPathways. In order to do that, a FAIR version of AOP-Wiki (the main AOP resource) and WikiPathways are to be created, and by utilizing RDF, they will be implemented in workflows. These workflows can be used, for example, to look up data for an AOP to support the biological plausibility, find AOPs related to experimental results, or identify the molecular pathways underlying the AOPs.¹



¹ <https://openrisknet.org/news/22/>

Webinar Report

AOP-DB: The Adverse Outcome Pathway Database

Date	2019-04-08
Presenters	Holly Mortensen, Ph.D. (US EPA), Phillip Langley (ORAU-SSC) and Trevor Levey (ORAU-SSC)
Website	https://openrisknet.org/events/60/
Webinar recording	https://youtu.be/DwLkbpccWS4
Slides	https://openrisknet.org/library/
Registrants	71
Attendees	51

The webinar presented the updated version of the EPA Adverse Outcome Pathway Database (AOP-DB), which includes an increased number of adverse outcomes and corresponding key events derived from direct integration of the AOPWiki XML. Aspects highlighted included how the database was originally envisioned, and case study examples of how the database can be used, as well as example queries using the development version of the AOP-DB frontend user interface. Further, the efforts underway to incorporate AOP-tissue specific network generation, and population-level characterization for AOP multilocus networks were also discussed.

The EPA Adverse Outcome Pathway Database (AOP-DB) is currently an internal EPA SQL database that supports discovery and development of putative and potential AOPs. The AOP-DB aggregates relationships between AOP-gene targets, chemical, disease, tissue, pathway, species orthology information, ontologies and gene interactions to characterize the impacts of chemicals to human health and the environment. The AOP-DB serves as a hypothesis generation and decision support tool for case study development. Associations are sourced from public annotation to provide biological context and are integrated with AOP information centralized in the AOP-Wiki. The AOP-DB allows for fast, automatic AOP profiling and exploration that gives a broad, systems-level overview of the biological context of AOPs, thus dramatically expediting predictive toxicology efforts. The long-term significance and impact of the AOP-DB tool is the continued translation of AOP biological context, and the ability to associate these data between and across AOPs, and with assay, chemical, and disease endpoints.

Webinar Report

How to describe OpenRiskNet services and their functionality by semantic annotation

Date	2019-05-13
Presenters	Thomas Exner (Edelweiss Connect GmbH, Switzerland)
Website	https://openrisknet.org/events/64/
Webinar recording	https://youtu.be/YD-ilh8lS0I
Slides	https://openrisknet.org/library/
Registrants	19
Attendees	14

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 first demonstrated 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 showed low level annotation, which are used for dataset and input/output harmonisation so that the user, but more importantly 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 were shown.

Webinar Report

Use of Nextflow tool for toxicogenomics-based prediction and mechanism identification in OpenRiskNet e-infrastructure

Date	2019-05-27
Presenters	Evan Floden (Fundacio Centre De Regulacio Genomica, Spain)
Website	https://openrisknet.org/events/65/
Webinar recording	https://youtu.be/JqYoZs3llpl
Slides	https://storage.googleapis.com/openrisknet/resources/2019/05/27/Presentation.pdf
Registrants	18
Attendees	11

Predictive toxicology and risk assessments increasingly rely on Big Data analyses for more informed decision making. Toxicogenomics uses transcriptomic readouts to predict the characteristics of compounds based on the gene-expression profiling of cells in response to exposure. These large genomic analysis place new computational demands on researchers with the handling of datasets, the combining of tools and the reproducible deployment of an analysis presenting significant challenges.

This webinar highlighted how these challenges can be overcome using the open source workflow management tool Nextflow within the OpenRiskNet e-infrastructure. Using the toxicogenomics example, we demonstrated how a workflow can be created, deployed and shared across Kubernetes-based environments.

To illustrate the use of external resources we developed a toxicogenomics use case that was also included in the webinar.¹



¹ <https://openrisknet.org/news/24/>

Webinar Report

Demonstration on OpenRiskNet approach on modelling for prediction or read across (ModelRX case study)

Date	2019-06-11
Presenters	Philip Doganis and Haralambos Sarimveis (National Technical University of Athens, Greece)
Website	https://openrisknet.org/events/67/
Webinar recording	https://youtu.be/yjYVNdUwHLg
Slides	https://storage.googleapis.com/openrisknet/resources/2019/06/24/ModelRX_Case_Study-Webinar_20190611.pdf
Registrants	23
Attendees	12

The ModelRX case study contributes to OpenRiskNet by providing computational methods to support suitability assessment of existing data and identification of analogues, and predictive modelling functionalities, which are essential in the field of final risk assessment.

During the webinar, we focused on the Jaqpot platform within the ModelRX case study. Starting from a dataset in Jaqpot v4 at <http://www.jaqpot.org>, we applied an algorithm to create a model and get predictions, which are accompanied by QPRF (QSAR prediction reporting format) report.

We also introduced the new Jaqpot v5 GUI (Graphical User Interface) at <https://app.jaqpot.org> that allows users easy upload of models they have developed in their own Python or R environment, make them available as web services and offers powerful sharing functionalities of online resources.

Webinar Report

Deploying Applications to an OpenRiskNet Virtual Environment

Date	2019-06-24
Presenters	Tim Dudgeon and Alan Christie (Informatics Matters Ltd, UK)
Website	https://openrisknet.org/events/66/
Webinar recording	https://youtu.be/qLgxaTPiKNc
Slides	https://storage.googleapis.com/openrisknet/resources/2019/06/24/Deploying_Applications_to_an_OpenRiskNet_Virtual_Environment.pdf
Registrants	18
Attendees	15

This webinar illustrated how the deployment of containerised services to an OpenRiskNet Virtual Environment is performed. Starting from a simple case of an existing container image that contains a service, such as one from Docker Hub, we demonstrated the process of deploying that service and configuring it so that it plays nicely with the Kubernetes environment and can be accessed by users and/or other services. Different approaches to deployment were discussed, as well as some more complex examples where multiple container images are involved.

- Brief introduction to OpenRiskNet Virtual Environments
- Brief introduction to OpenShift
- Brief introduction to containers
- Approaches to deploying a single container image (example: Lazar, BridgeDB)
 - Through console
 - Through CLI
 - Using OpenShift templates
 - Using Template Service Broker
- Deploying a more complex multi-container application (example: Squonk)
- Summary

From this webinar it is expected that the attendees have the basic knowledge to get started on deploying their own containerised services.

Webinar Report

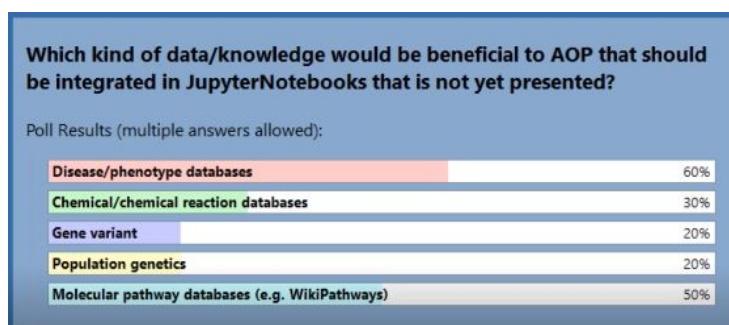
Connecting Adverse Outcome Pathways, knowledge and data with AOPLink workflows

Date	2019-07-15
Presenters	Marvin Martens (Department of Bioinformatics, Maastricht University, The Netherlands)
Website	https://openrisknet.org/events/70/
Webinar recording	https://youtu.be/hbINApnhubM
Slides	https://storage.googleapis.com/openrisknet/resources/2019/07/15/Slides_webinar_AOPLink_15-07-2019.pdf
Registrants	23
Attendees	18

This webinar is a follow-up of the previous “[Identification and linking of data related to AOPWiki \(an OpenRiskNet case study\)](#)” webinar on March 26th, in which the OpenRiskNet project and AOPLink case study were introduced.

The objectives of the AOPLink case study are to explore Adverse Outcome Pathway (AOP) knowledge, and the validation and linking of existing knowledge to support AOPs. Another goal is the establishment of links between AOPs and experimental data to support the biological plausibility of Key Events, and identify Key Events based on an experimental dataset.

The central component in this case study is the RDF-converted AOP-Wiki, the main repository for qualitative AOPs. The RDF is exposed in a SPARQL endpoint and with an API that allows us to ask a wide variety of questions. This webinar will highlight the functionalities of the AOP-Wiki SPARQL endpoint, demonstrated with several example queries to extract specific information from the database. Also, federated queries between the AOP-Wiki RDF with SPARQL endpoints of other databases, such as Rhea, DisGeNET, and WikiPathways, will be shown.



In order to answer the main research questions of the AOPLink case study, the AOP-Wiki SPARQL endpoint is used in Jupyter notebooks to find data related to AOPs in a variety of databases, and extend the knowledge that is captured in the AOP-Wiki. Furthermore, a notebook on nanomaterial-related AOP identification will be shown, and the near future of the AOPLink case study will be described for the final months of the OpenRiskNet project.

OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE

Workshop

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

23-24 October 2019 (Amsterdam, The Netherlands)



This project is funded by the European Union

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

Project identification

Grant Agreement	731075
Project Name	OpenRiskNet: Open e-Infrastructure to Support Data Sharing, Knowledge Integration and <i>in silico</i> Analysis and Modelling in Risk Assessment
Project Acronym	OpenRiskNet
Project Coordinator	Edelweiss Connect GmbH
Star date	1 December 2016
End date	30 November 2019
Duration	36 Months

OpenRiskNet Consortium



EwC = Edelweiss Connect GmbH, Switzerland
JGU = Johannes Gutenberg-Universität Mainz, Germany
CRG = Fundacio Centre De Regulacio Genomica, Spain
UM = Universiteit Maastricht, Netherlands
UoB = The University Of Birmingham, United Kingdom
NTUA = National Technical University Of Athens, Greece
Fraunhofer = Fraunhofer Gesellschaft Zur Foerderung Der Angewandten Forschung E.V., Germany
UU = Uppsala Universitet, Sweden
IM = Informatics Matters Limited, United Kingdom
INERIS = Institut National De L'environnement Et Des Risques INERIS, France
VU = Vrije Universiteit Amsterdam, Netherlands

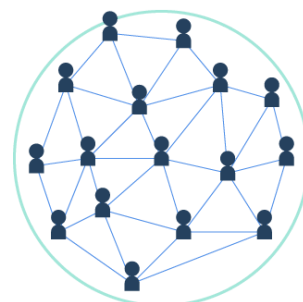
Table of Contents

WELCOME NOTE	4
RESOURCES FOR PARTICIPANTS	5
AGENDA	6
Day 1 - 23 October 2019	6
Day 2 - 24 October 2019	7
ABSTRACTS	9
Lectures and demonstrations	9
Adoption of OpenRiskNet solutions by NanoSafety community and NanoCommons infrastructure	9
The European Open Science Cloud, its implementation projects (eInfraCentral, OpenAIRE and EOSC-hub) and the EOSC Portal	10
ToxicoGx - An R platform for integrated toxicogenomics data analysis	11
Using SPARQL to explore human protein data in neXtProt and beyond	11
Strategy used to build confidence in PROSILICO's in silico methods for prediction of human clinical ADME/PK	12
FAME 3: Predicting the Sites of Metabolism in Small Molecules for Phase 1 and Phase 2 Metabolic Enzymes	13
US EPA AOP-DB: A database resource for the exploration of Adverse Outcome Pathways	13
ToxPlanet	14
Posters	15
The NanoCommons e-infrastructure – A quick guide to what and how of nanoinformatics in safety assessment suiting basic to expert users in academia, industry, and regulatory agencies	15
The BridgeDb framework: new functionality and integrations	16
A network-based approach for predicting key events and transcription regulators associated with nanomaterial-induced toxicity	16
Development of an API for the Site of Metabolism Predictor FAME 3	17
OpenRiskNet Part I: Development of an open e-infrastructure predictive toxicology and risk assessment	18
OpenRiskNet Part II: Predictive Toxicology based on Adverse Outcome Pathways and Biological Pathway Analysis	19
OpenRiskNet Part III: Modelling Services in Chemical/Nano-safety, Environmental Science and Pharmacokinetics	20
OpenRiskNet Part IV: WEKA Machine Learning Services for the Prediction of Half-Lives of Chemicals and Nanoparticle Transport	20
LOGISTICS	22
Venue	22
Recommended hotels	22

WELCOME NOTE

The **OpenRiskNet** project, developing and implementing an open e-infrastructure addressed to research and industrial communities performing risk assessment of consumer products like chemicals, cosmetics or drugs, is in its third and final year.

To disseminate the achievements and implemented concepts of the project, make the stakeholders aware of the solutions developed, find the best options for the adoption by other projects or organisations, a final workshop is organized. The event will create the perfect environment for current and future users of OpenRiskNet services, developer and administrators as well as the members of related (e-)infrastructure communities to interact with OpenRiskNet developers, modellers and project managers, learn more about the success of the community building efforts fostered by the associated partner programme and the implementation challenges, establish and strengthen links to other projects and organize the transfer of the technology into these.



The workshop is addressing all OpenRiskNet stakeholders (scientific, industrial and regulatory communities) that are invited to participate in this interactive event. This will ensure that all relevant and target groups that need to be aware of the project achievements have access to this information and are enabled to give feedback, and also be trained on the provided solutions.

Therefore we invite members of research organisations, academia, regulators and governmental agencies, SMEs and CROs, members of EU infrastructure initiatives to join us for the final workshop. Besides researchers, risk assessors and regulators, the workshop is specifically designed to provide the needed information for developers on how to integrate additional services and for system administrators on deployment options of the virtual research environments in parallel sessions.

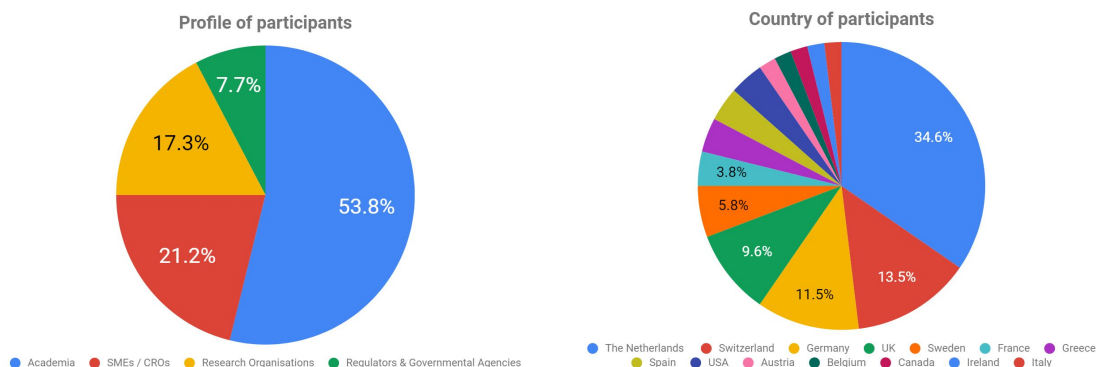
A significant part of the event (day 1) will focus on the [case studies](#), demonstrations and hands-on training sessions, where the teams involved in the development and implementation will present and demonstrate the use of the services included in the OpenRiskNet e-infrastructure.

Day 2 will then focus on the outreach and sustainability aspects:

- 1) The [implementation challenges](#) were implemented as an innovative part of the [associated partners](#) programme during the project and linked ten new organisations intensively to project as service providers and early adopters. Complementary services from these partners can now be used and were integrated in the case studies workflow.

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

- 2) The **sustainability** measures, the support and maintenance of the infrastructure after the end of the project, collaborations and links created with other communities will be highlighted and discussed with representatives of other major pan-European infrastructures and policy makers.



RESOURCES FOR PARTICIPANTS

- Case studies description: <https://openrisknet.org/e-infrastructure/development/case-studies/>
- Training materials <https://openrisknet.org/library/>
- E-infrastructure reference site <https://home.prod.openrisknet.org/>
- GitHub repository: <https://github.com/OpenRiskNet>

AGENDA

Day 1 - 23 October 2019

8:30-9:00	<i>Registration</i>	
9:00-9:10	Welcome and introduction to the workshop	<i>Thomas Exner (Edelweiss Connect, GmbH, Switzerland)</i>
9:10-9:30	OpenRiskNet Case studies introduction and concept	<i>Paul Jennings (Vrije Universiteit Amsterdam, The Netherlands)</i>
9:30-10:30 <i>8 min / case study</i>	OpenRiskNet Case studies (flash presentations): <ul style="list-style-type: none"> • DataCure - Thomas Exner (EwC) • ModelRX - Philip Doganis (NTUA) • TGX - Danyel Jennen (UM) • SysGroup - Danyel Jennen (UM) • MetaP - Daan Geerke (VU) • AOPLink - Marvin Martens (UM) • RevK - Philip Doganis (NTUA) 	
10:30-11:00	<i>Coffee break (incl. posters viewing)</i>	
OpenRiskNet demo & training sessions		
11:00-12:30	<ul style="list-style-type: none"> • Workflows: practical example of Jupyter notebooks use, Data curation example, workflow across multiple case studies 	<i>Marvin Martens (UM) Thomas Exner (EwC)</i>
12:30-13:30	<i>Lunch break</i>	
13:30-15:00	Parallel sessions: <ul style="list-style-type: none"> • Group 1: Deploying Applications (addressed to developers, services providers and infrastructure admins) (<u>Room: 12W24</u>) • Group 2: Modelling exercise (built around the ModelRX case study, support of the DataCure) (addressed to end-users) (<u>Room: 01W08</u>) 	<i>Tim Dudgeon (IM)</i> <i>Philip Doganis and Pantelis Karatzas (NTUA) Denis Gebele (JGU) Tomaž Mohorič (EwC) Jonathan Alvarsson (UU)</i>
15:30-16:00	<i>Coffee break (incl. posters viewing)</i>	
16:00-17:30	Parallel sessions: <ul style="list-style-type: none"> • Group 1: Q&A Deploying Applications (<u>Room: 12W24</u>) 	<i>Tim Dudgeon (IM)</i>

	<ul style="list-style-type: none"> Group 2: Ontology and semantic annotations (Room: 01W08) 	Egon Willighagen (UM)
18:00-	Dinner - Buffet organised at workshop venue	

Day 2 - 24 October 2019

Associated partners session		
Chair: Rex FitzGerald (Swiss Centre for Applied Human Toxicology, University of Basel, Switzerland)		
9:00-10:45 20 min / presentation	Strategy used to build confidence in PROSILICO's <i>in silico</i> methods for prediction of human clinical ADME/PK	Urban Fagerholm (Prosilico, Sweden)
	FAME 3: Predicting the Sites of Metabolism in Small Molecules for Phase 1 and Phase 2 Metabolic Enzymes	Johannes Kirchmair (University of Hamburg, Germany)
	Using SPARQL to explore human protein data in neXtProt and beyond	Lydie Lane (CALIPHO group, SIB Swiss Institute of Bioinformatics, Switzerland)
	ToxicoGx: An R platform for integrated toxicogenomics data analysis	Sisira Kadambat Nair (Princess Margaret Cancer Centre, University Health Network, Toronto, Canada)
	US EPA AOP-DB: A database resource for the exploration of Adverse Outcome Pathways	Holly M. Mortensen (US Environmental Protection Agency, Office of Research and Development, USA)
10:45-11:15	Coffee break (incl. posters viewing)	
11:15-12:00	ToxPlanet: demo, information on API, discussion on use case scenarios	Matt Timberlake (ToxPlanet, USA)
12:00-12:15	Diamond Light Source: OpenRiskNet's first external Virtual Environment	Tim Dudgeon (Informatics Matters Ltd, UK)
12:15-12:30	Lessons learned from the associated partner programme	Thomas Exner (Edelweiss Connect GmbH, Switzerland)
12:30-13:30	Lunch break	

EU infrastructures & sustainability session		
Chair: Stefan Kramer (Johannes Gutenberg University Mainz, Germany)		
13:30-14:00	Adoption of OpenRisknet solutions by NanoSafety community and NanoCommons infrastructure	<i>Iseult Lynch (University of Birmingham, UK)</i>
14:00-15:00	1. Introduction to the European Open Science Cloud (EOSC) (10 min)	<i>Alessia Bardi (Institute of Science and Technology of Information, CNR, Italy)</i>
	2. OpenAIRE : an EOSC implementation project (10 min)	
	3. eInfraCentral : an EOSC implementation project (10 min)	<i>Bjorn Backeberg (EGI Foundation, The Netherlands) on behalf of Jelena Angelis (EFIS Centre, Belgium)</i>
	4. EOSC-hub : an EOSC implementation project (10 min)	<i>Bjorn Backeberg (EGI Foundation, The Netherlands)</i>
	5. Technical demo of cloud and storage services in EOSC (20 min)	<i>Yin Chen (EGI Foundation, The Netherlands)</i>
15:00-15:30	<i>Coffee break</i>	
15:30-16:00	Panel discussion: lesson learned and looking ahead to the next steps	
16:00-16:15	Closing session	

ABSTRACTS

Lectures and demonstrations

Adoption of OpenRiskNet solutions by NanoSafety community and NanoCommons infrastructure

Iseult Lynch

School of Geography, Earth and Environmental Sciences, University of Birmingham, UK

Nanomaterials present a unique set of challenges and opportunities for scientists and regulators, arising from quantum confinement (e.g. novel electronic properties, band-gaps that overlap with cells, etc.), and their enormous reactive surface area that leads to agglomeration and binding to biomolecules. Other challenges include the well-known difficulties in terms of batch-to-batch variability in many nanomaterials synthesis or production routes, and the dynamic nature of nanomaterials themselves, whereby ageing can occur during storage and transformations occur upon contact with biological or environmental matrices. Despite these differences, much can be learned from classical toxicology and pharmacology and from the chemoinformatics approaches applied to chemicals. Indeed, it is fully understood that the toxicity pathways and adverse outcomes induced by nanomaterials are not unique to nanomaterials, although the molecular initiating events may be (nano)particle-specific such as surface-generated reactive oxidative species or surface-binding related protein unfolding resulting from corona formation, for example. Thus, the nanosafety community strives to build upon, and leverage, developments from chemoinformatics where possible and adapt for nanomaterials, in the same way it is adapting the regulatory testing guidelines to account for non-equilibrium conditions and non-soluble nanomaterials.

OpenRiskNet aimed to leverage commonalities in approaches across different classes of chemicals, and to develop modular scalable solutions. It focussed on process-based solution, including containerization (e.g. Docker), semantic query language for databases (SPARQL), and integration of a range of chemoinformatics tools for AOP and PBPK modelling via Jupyter notebooks, for example.

Starting as it did 18 months after OpenRiskNet, NanoCommons has been leveraging many of the OpenRiskNet advances, and building on its experiences. For example, OpenRiskNet had to do considerable work around ethics of *in vivo* datasets generated by others and to understand their responsibilities as data hosts / providers. The approaches taken, whereby ethics statements and licence information is included as part of the initial information gathering step from potential dataset providers, and ethics information is included as part of the data and metadata, is adopted in NanoCommons for all datasets curated and imported. OpenRiskNet also developed a searchable Services catalogue approach, allowing the standardised documentation of all services its provides, both those generated by partners

and associated partners as well as services added by external providers, that can be searched and filtered by the category of service, the service type, the user type (developers, end-users, system admin) and the targeted user (e.g. informed public through regulator to data manager). This system, and the services developed, are incorporated into NanoCommons now, as most of the tools developed are also applicable to nanomaterials, or can be further developed as case studies within NanoCommons for use with nanomaterials.

As part of its long-term sustainability planning, NanoCommons is working closely with the European Union Observatory for Nanomaterials (EUON) to understand how best to integrate the NanoCommons Knowledge base and its associated nanoinformatics and risk assessment tools, into the EUON platform, which aims to provide increased transparency regarding the safety of nanomaterials and nano-enabled products. Other sustainability activities underway, co-developed by OpenRiskNet and NanoCommons include working with Elixir to develop a toxicology (including nanotoxicology) community, and more recently to implement Bioschemas annotation for toxicology.

The European Open Science Cloud, its implementation projects (eInfraCentral, OpenAIRE and EOSC-hub) and the EOSC Portal

Alessia Bardi¹ (OpenAIRE), Jelena Angelis² (eInfraCentral), Yin Chen³ (EOSC-hub), Gergely Sipos³ (EOSC-hub), Björn Backeberg³ (EOSC-hub)

¹Institute of Science and Technology of Information, CNR, Italy; ²EFIS Centre, Belgium; ³EGI Foundation, The Netherlands

In recent years, the vision of Open Science has emerged as a new paradigm for transparent, data-driven science capable of accelerating competitiveness and innovation. The embodiment of this vision in Europe is the European Open Science Cloud (EOSC), first proposed by the European Commission in April 2016 as part of the Communication on the 'European Cloud Initiative', one of the pillars of the Digital Single Market Strategy. The EOSC puts into practice the European vision for Open Innovation, Open Science and Open to the World by bringing together services and research products such as computing, storage, data, publications, software and workflows from national and international research infrastructures, research performing organisations, collaborations and projects. In so doing, EOSC aims to position Europe as a global leader in scientific data infrastructures and to ensure that European scientists reap the full benefits of data-driven science. The EOSC will offer a virtual environment with open and seamless services for storage, management, analysis and re-use of research data, across borders and scientific disciplines.

Implementation projects such as eInfraCentral, OpenAIRE and EOSC-hub, play central roles in implementing the EOSC vision. The European Commission described them in the Implementation Roadmap for the European Open Science Cloud among the key building blocks of EOSC. The projects bring mature processes, policies and tools from the leading European e-infrastructures to manage the entire life-cycle of services into EOSC, from design to delivery. The entry point into EOSC is the EOSC Portal: <http://www.eosc-portal.eu>. Here researchers can discover, order, access, use and reuse the services, analytical tools, data

management tools, storage and computing resources they need for their work. Service providers can advertise their services and resources in the portal to make them discoverable and available for access to a broader user group. In this session we present the EOSC vision for open science, the EOSC supporting initiatives, including its implementation projects.

The EOSC Portal is jointly developed and maintained by current EOSC implementation projects: eInfraCentral, EOSC-hub, EOSCpilot and OpenAIRE-Advance.

ToxicoGx - An R platform for integrated toxicogenomics data analysis

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To better understand the molecular mechanisms underlying compound toxicity, great efforts have been made in screening of drugs/chemicals to generate datasets such as Open-TG GATEs and DrugMatrix. These datasets generate molecular and pharmacological profiles several tissues including liver and kidney along with histopathology assessment and curated literature annotations both in in vivo and in vitro settings. Even though the importance of these datasets is unequivocal, it is important to integrate data across multiple models with maximum overlap and consistency. Some of the major challenges in carrying out comparative analysis of these datasets are the differences in experimental set-up across laboratories and drug annotations, hindering research reproducibility. We have developed ToxicoGx, an open source R package to facilitate integrative analysis of these datasets with intersecting functions that would allow identification of robust biomarkers. A ToxicoSet (TSet) efficiently stores molecular and drug response data along with experimental metadata. It can be easily downloaded and used for data visualization and analyses such as plotting dose response curves, identify differential gene expression induced by drug treatment, and checking gene-compound associations. A detailed tour of the package will be demonstrated in the presentation using knitr (Vignette).

Using SPARQL to explore human protein data in neXtProt and beyond

Lydie Lane and the neXtProt team

SIB Swiss Institute of Bioinformatics and University of Geneva, Geneva, Switzerland

The neXtProt platform (www.nextprot.org) developed at SIB Swiss Institute of Bioinformatics - the Swiss ELIXIR node - proposes solutions to select, explore and reuse available data on human proteins.

The neXtProt team manually curates data from the literature (post-translational modifications, variant phenotypes, protein-protein interactions, etc.) and combines it with

high quality data generated by systems biology projects using a single inter-operable format, the RDF (Resource Description Framework) format. neXtProt data are FAIR (Findable, Accessible, Interoperable, and Reusable), with full traceability ensured by extensive use of metadata.

In the last four years, we have been promoting the use of SPARQL (SPARQL Protocol & RDF Query Language), a semantic query language for databases. Given the wealth of data in neXtProt, our data model is quite complex. neXtProt thus provides over 150 pre-built queries and documentation of its data model to guide the user in his or her first steps. The power and exquisite preciseness of the SPARQL language allow users to simultaneously explore data from neXtProt and data from other semantically compatible resources such as UniProtKB, ChEMBL, DrugBank, Rhea, PDB or WikiPathways.

We would be glad to discuss how we could federate neXtProt data with data from OpenRiskNet resources to benefit risk assessment studies.

Strategy used to build confidence in PROSILICO's in silico methods for prediction of human clinical ADME/PK

Urban Fagerholm and Sven Hellberg

PROSILICO, Sweden

Animal data-based models have been, and still are, the golden standard for predicting ADME/PK and doses of drug candidates in early clinical studies. In vitro models have been developed and are also applied for such predictions. These have apparent advantages and are now accepted as complements to or replacements of animal models. Among limitations of these in vitro systems are a poorer overall predictive accuracy and limited application domain and a belief that simpler systems should not be able outperform those with higher complexity (such as a whole body animal model). Predictive in silico methods have also been developed, and these are mainly applied for screening purposes. Their predictive accuracy and range have not reached those of lab methods. In order to replace lab methods these not only need to show superiority or similar predictive quality, but also a changed mind-set (that a computational model actually can be more reliable than lab methods). PROSILICO has developed an integrated in silico-based platform, including software, for prediction of ADME/PK and doses in humans that outperforms labs in both accuracy and range, and appears to be first to offer a service that can compete with labs. During the talk the strategy used for building this unique predictive platform and confidence in it will be demonstrated.

FAME 3: Predicting the Sites of Metabolism in Small Molecules for Phase 1 and Phase 2 Metabolic Enzymes

Martin Šícho^{1,2}, Conrad Stork¹, Angelica Mazzolari³, Christina de Bruyn Kops¹, Alessandro Pedretti³, Bernard Testa⁴, Giulio Vistoli³, Daniel Svozil², Johannes Kirchmair^{1,5,6}

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In silico models for predicting the atoms in a molecule at which metabolic reactions are initiated (sites of metabolism) can help enormously in the development of strategies for the optimization of bioactive compounds. In this contribution we report on the development of the third generation of FAsT MEtabolizer (FAME 3), a predictor of sites of metabolism that is based on a collection of extra trees classifiers. FAME 3 is trained on data extracted from the recently launched MetaQSAR database, a comprehensive resource of expert-curated data on xenobiotic metabolism. FAME 3 is one of only a few predictors that cover a wide range of phase 1 and phase 2 metabolic reactions. Benchmark studies on holdout data show that FAME 3 reaches competitive performance. Importantly, FAME 3 features a new, atom-based distance measure that provides an estimate of the reliability of predictions for each atom in a molecule of interest. An API for the OpenRiskNet infrastructure is currently under development.

US EPA AOP-DB: A database resource for the exploration of Adverse Outcome Pathways

Holly M. Mortensen¹, Trevor Levey²

¹US Environmental Protection Agency, Office of Research and Development (ORD), National Health and Environmental Effects Laboratory, Research Triangle Park, NC 27709, USA; ²Oak Ridge Associated Universities, Research Triangle Park, NC 27709, USA.

There is a need for approaches to understand the biological mechanism of adverse outcomes and human variability in response to environmental chemical exposure. The EPA Adverse Outcome Pathway Database (AOP-DB) is a database resource that combines different data types (AOP, gene, chemical, disease, pathway, orthology, and ontology) to characterize the impacts of chemicals to human health and the environment, and serves as a decision support tool for case study development. Here we present an updated version of the database, which includes an increased number of adverse outcomes and corresponding key events derived from updated feeds from the AOP-Wiki (<https://aopwiki.org/>), updated disease, phenotype, and ontology information, as well as improved integration with the AOP-DB web user interface. We illustrate these updates and the utility of the AOP-DB through

modules which provide the user with opportunities to explore computationally how chemical-gene molecular key events in adverse outcome pathways link to adverse disease, tissue-specific and population-level health outcomes. This abstract does not reflect EPA Policy.

ToxPlanet

Matt Timberlake

ToxPlanet, USA

Over the last 15+ years, ToxPlanet has assembled and curated hundreds of freely-available high-quality databases available from government agencies, NGO's, and other interested groups. Our AWS-hosted collection, now containing several million documents covering nearly 1 million chemicals, can be accessed using our ORN-compliant API and integrated with additional tools and services. This presentation will include a presentation of the ToxPlanet website, information on our API, and a discussion on current and potential use cases.

Posters

The NanoCommons e-infrastructure – A quick guide to what and how of nanoinformatics in safety assessment suiting basic to expert users in academia, industry, and regulatory agencies

Martin Himly¹, Lucian Farcal², Anastasios Papadiamantis³, Albert Duschl¹, Iseult Lynch³ and the NanoCommons consortium

¹University of Salzburg, Austria; ²Edelweiss Connect GmbH, Basel, Switzerland; ³University Of Birmingham, United Kingdom;

NanoCommons (<https://www.nanocommons.eu/>) is a research e-infrastructure project offering access to high quality nanoinformatics services for nanosafety assessors in academia, industry, regulatory agencies. It is user-led, offering and developing the services needed by the user community of nanotechnology, nanosafety and related fields. NanoCommons is built on 3 main pillars: joint research activities, networking activities and transnational access services, covering four categories relevant for nanosafety assessment:

- experimental workflows design and implementation;
- data processing and analysis;
- data visualisation and predictive toxicity;
- data storage and online accessibility.

These services are designed to promote data FAIRness (Findable, Accessible, Interoperable, and Reusable), a key NanoCommons goal, that can be made Open through the NanoCommons Knowledgebase. Thus, NanoCommons provides innovative solutions for data mining, harmonisation, utilisation and re-utilisation, including incorporation of a range of modelling and decision support tools that require and/or can produce organised, high-quality datasets. A number of online training tools have been developed for each of the offered services to help users choose the services relevant to their research questions and applications. The NanoCommons infrastructure encompassing a training library shall bridge academic research with industry and regulators, as recommended by the EU NanoSafety Cluster's "Closer to the Market" Research Roadmap serving the Safe-by-Design concept in nanotechnology.

This work is funded by the European Union's H2020 Research & Innovation Action „NanoCommons – The European Nanotechnology Community Informatics Platform: Bridging data and disciplinary gaps for industry and regulators“ (grant agreement No 731032).

The BridgeDb framework: new functionality and integrations

Egon Willighagen, The BridgeDb Project

Department of Bioinformatics - BiGCaT, Maastricht University, The Netherlands

Biological systems consist of many thousands of genes, proteins, and metabolites. Our collective knowledge about these entities is collected in many hundreds of disparate databases, each focusing on particular themes of knowledge or types of experiments. Importantly, to capture this focus, each database uses its own definition of the key entities and have a matching collection of entity identifiers. Linking all these identifiers requires a flexible tool that provides identifier mappings (IDmaps) but that also knows about these complexities. BridgeDb (<http://bridgedb.org>) offer IDmaps and understands the difference between a gene, a DNA sequence, a microarray probe, and a protein. Likewise, it understands the difference between stereoisomers, protonation states, and compound classes for metabolites and other small molecules. Modules and plugins are available to use BridgeDb in many bioinformatics toolsets. Furthermore, the latest version fully supports the Linked Open Data Cloud. The BridgeDb project involves developers from Maastricht University, the Netherlands Cancer Institute, and Manchester University, and collaborates with, for example, the Gladstone Institutes, Heriot-Watt University, and Uppsala University.

A network-based approach for predicting key events and transcription regulators associated with nanomaterial-induced toxicity

Vadim Zhernovkov¹, Tapesh Santra¹, Hilary Cassidy¹, Oleksii Rukhlenko¹, David Matallanas², Aleksandar Krstic¹, Walter Kolch^{1,2,3}, Vladimir Lobaskin⁴, and Boris N. Kholodenko^{1,2,3,5}

¹Systems Biology Ireland, University College Dublin, Dublin 4, Ireland; ²School of Medicine and Medical Science, University College Dublin, Belfield, Dublin 4, Ireland; ³Conway Institute of Biomolecular & Biomedical Research, University College Dublin, Ireland; ⁴School of Physics, University College Dublin, Dublin 4, Ireland; ⁵Department of Pharmacology, Yale University School of Medicine, New Haven CT 06520, USA

A rapid increase of new nanomaterial (NM) products poses new challenges for their risk assessment. Current traditional methods for estimating potential adverse health effect of NMs are complex, time consuming, and expensive. In order to develop new prediction tests for nanotoxicity evaluation, a systems biology approach, and data from high-throughput omics experiments can be used. We present a computational approach that combines reverse engineering techniques, network analysis and pathway enrichment analysis for inferring the transcriptional regulation landscape and its functional interpretation. To illustrate this approach, we used published transcriptomic data derived from mice lung tissue exposed to carbon nanotubes (NM-401 and NRCWE-26). Because fibrosis is the most common adverse effect of these NMs, we included in our analysis the data for bleomycin (BLM) treatment, which is a well-known fibrosis inducer. We inferred gene regulatory networks for each NM and BLM to capture functional hierarchical regulatory structures between genes and their regulators. Despite the different nature of the lung injury caused by nanoparticles and BLM, we identified several conserved core regulators for all agents. We reason that these regulators can be considered as early predictors of toxic responses after

NMs exposure. This integrative approach, which refines traditional methods of transcriptomic analysis, can be useful for prioritization of potential core regulators and generation of new hypothesis about mechanisms of nanoparticles toxicity.

Development of an API for the Site of Metabolism Predictor FAME 3

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An important factor to consider in risk assessment is the metabolic fate of xenobiotics. In this endeavor, the availability of a software tool to accurately predict sites of metabolism (atoms in a molecule at which metabolic reactions are initiated) would help to speed up the process of understanding a compound's metabolism and dramatically reduce experimental costs. FAME 3 [1] is the last iteration of FAsT METabolizer, a site of metabolism predictor utilizing random forest classifiers and atom descriptors. Based on a large expert-curated data set (MetaQSAR [2]), FAME 3 is one of few predictors that cover both phase 1 and phase 2 metabolic reactions and, unlike other predictors, features an estimate of the reliability of individual SoM predictions. In this work, we briefly describe the relevant features of FAME 3, but more importantly we focus on the specification and usage examples of the FAME 3 application programming interface (API) that is currently being implemented within the OpenRiskNet infrastructure. FAME 3 and its OpenRiskNet API are free for academic and noncommercial research, and this work should serve as a guide to anyone who would like to use this software for not only risk assessment, but also in any other context.

References

1. FAME 3: Predicting the Sites of Metabolism in Synthetic Compounds and Natural Products for Phase 1 and Phase 2 Metabolic Enzymes Martin Šícho, Conrad Stork, Angelica Mazzolari, Christina de Bruyn Kops, Alessandro Pedretti, Bernard Testa, Giulio Vistoli, Daniel Svozil, and Johannes Kirchmair *Journal of Chemical Information and Modeling* 2019 59 (8), 3400-3412 DOI: 10.1021/acs.jcim.9b00376
2. MetaQSAR: An Integrated Database Engine to Manage and Analyze Metabolic Data Alessandro Pedretti, Angelica Mazzolari, Giulio Vistoli, and Bernard Testa *Journal of Medicinal Chemistry* 2018 61 (3), 1019-1030 DOI: 10.1021/acs.jmedchem.7b01473

OpenRiskNet Part I: Development of an open e-infrastructure predictive toxicology and risk assessment

Thomas Exner¹, Lucian Farcal¹, Daniel Bachler¹, Nofisat Oki¹, Denis Gebele², Atif Raza², Stefan Kramer², Evan Floden³, Cedric Notredam³, Jordi Rambla³, Danyel Jennen⁴, Jumamurat Bayjanov⁴, Egon Willighagen⁴, Marvin Martens⁴, Chris Evelo⁴, Iseult Lynch⁵, George Gkoutos⁵, Philip Doganis⁶, Pantelis Karatzas⁶, Haralambos Sarimveis⁶, Marc Jacobs⁷, Ola Spjuth⁸, Tim Dudgeon⁹, Alan Christie⁹, Frederic Bois¹⁰, Daan Geerke¹¹, Paul Jennings¹¹, Barry Hardy¹

¹Edelweiss Connect GmbH, Basel, Switzerland; ²Johannes Gutenberg-Universität Mainz, Germany; ³Fundacio Centre De Regulacio Genomica, Spain; ⁴Maastricht University, Netherlands; ⁵University Of Birmingham, United Kingdom; ⁶National Technical University Of Athens, Greece; ⁷Fraunhofer Gesellschaft, Germany; ⁸Uppsala Universitet, Sweden; ⁹Informatics Matters Ltd., United Kingdom; ¹⁰Institut National De L'environnement Et Des Risques, France; ¹¹Vrije Universiteit Amsterdam, Netherlands.

OpenRiskNet (<https://openrisknet.org/>) is a 3-year project funded by the EU within Horizon 2020 EINFRA-22-2016 Programme, with the main objective to develop an open e-infrastructure providing data and software resources and services to a variety of industries requiring risk assessment (e.g. chemicals, cosmetic ingredients, pharma or nanotechnologies).

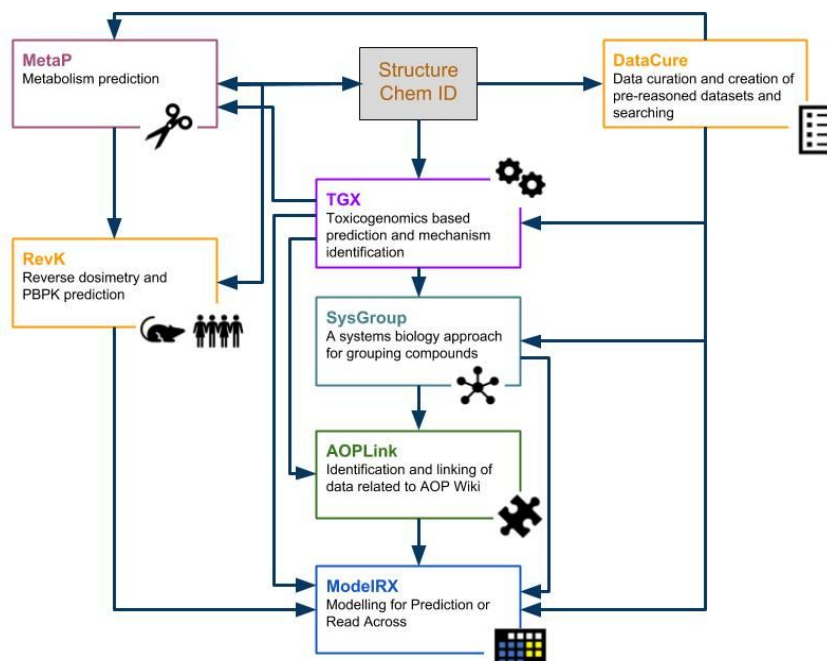


Figure 1. Structure of interlinked case studies targeting different parts of the risk assessment workflow

The infrastructure is built on virtual research environments (VREs), which can be deployed to workstations as well as public and in-house cloud infrastructures. Services providing data, data analysis, modelling and simulation tools for risk assessment are integrated into the

e-infrastructure and can be combined into workflows using harmonised and interoperable application programming interfaces (APIs) (<https://openrisknet.org/e-infrastructure/services/>). For complete risk assessment and safe-by-design studies, OpenRiskNet e-infrastructure functionality is combined via a variety of incorporated services demonstrated within a set of case studies (see figure 1). The case studies present real-world settings such as data curation, systems biology approaches for grouping compounds, read-across applications using chemical and biological similarity, and identification of areas of concern based only on alternative methods (non-animal testing) approaches.

OpenRiskNet is working with a network of partners, organised within an Associated Partners Programme, aiming to strengthen the working ties to other organisations developing relevant solutions or tools.

OpenRiskNet Part II: Predictive Toxicology based on Adverse Outcome Pathways and Biological Pathway Analysis

Marvin Martens¹, Thomas Exner², Nofisat Oki², Danyel Jennen¹, Jumamurat Bayjanov¹, Chris Evelo¹, Tim Dudgeon³, Egon Willighagen¹

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The OpenRiskNet project (<https://openrisknet.org/>) is funded by the H2020-EINFRA-22-2016 Programme.

Here we present how the concept of Adverse Outcome Pathways (AOPs), which captures mechanistic knowledge from a chemical exposure causing a Molecular Initiating Event (MIE), through Key Events (KEs) towards an Adverse Outcome (AO), can be extended with additional knowledge by using tools and data available through the OpenRiskNet e-Infrastructure. This poster describes how the case study of AOPLink, together with DataCure, TGX, and SysGroup, can utilize the AOP framework for knowledge and data integration to support risk assessments. AOPLink involves the integration of knowledge captured in AOPs with additional data sources and experimental data from DataCure. TGX feeds this integration with prediction models of the MIE of such AOPs using either gene expression data or knowledge about stress response pathways. This is complemented by SysGroup, which is about the grouping of chemical compounds based on structural similarity and mode of action based on omics data. Therefore, the combination of these case studies extends the AOP knowledge and allows biological pathway analysis in the context of AOPs, by combining experimental data and the molecular knowledge that is captured in KEs of AOPs.

OpenRiskNet Part III: Modelling Services in Chemical/Nano-safety, Environmental Science and Pharmacokinetics

Stefan Kramer¹, Philip Doganis², Denis Gebele¹, Atif Raza¹, Pantelis Karatzas², Haralambos Sarimveis², Jonathan Alvarsson³, Ola Spjuth³, Staffan Arvidsson³, Thomas Exner⁴, Lucian Farcas⁴, Barry Hardy⁴ for the OpenRisknet Consortium

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The OpenRiskNet project (<https://openrisknet.org/>) is funded by the H2020-EINFRA-22-2016 Programme and its main objective is the development of an open e-infrastructure providing data and software resources and services to a variety of industries requiring risk assessment (e.g. chemicals, cosmetic ingredients, pharma or nanotechnologies).

The concept of case studies was followed in order to test and evaluate proposed solutions and is described in <https://openrisknet.org/e-infrastructure/development/case-studies/>. Two case studies, namely ModelRX and RevK, focus on modelling within risk assessment.

The ModelRX – Modelling for Prediction or Read Across case study provides computational methods for predictive modelling and support of existing data suitability assessment. It supports final risk assessment by providing calculations of theoretical descriptors, gap filling of incomplete datasets. computational modelling (QSAR) and predictions of adverse effects. Services are offered through Jaqpot (UI/API), JGU WEKA (API), Lazar (UI) and Jupyter & Squonk Notebooks.

In the RevK – Reverse dosimetry and PBPK prediction case study, physiologically based pharmacokinetic (PBPK) models are made accessible for the purpose of risk assessment-relevant scenarios. The PKSim software, the httk R package and custom-made PBPK models have been integrated. RevK offers services through Jaqpot (UI/API).

OpenRiskNet Part IV: WEKA Machine Learning Services for the Prediction of Half-Lives of Chemicals and Nanoparticle Transport

Stefan Kramer, Denis Gebele, Atif Raza

Johannes Gutenberg-Universität Mainz, Germany

The OpenRiskNet project (<https://openrisknet.org/>) is funded by the H2020-EINFRA-22-2016 Programme and its main objective is the development of an open e-infrastructure providing data and software resources and services to a variety of industries requiring risk assessment (e.g. chemicals, cosmetic ingredients, pharma or nanotechnologies).

We will present the WEKA machine learning services within the infrastructure and how they can be used to solve complex prediction tasks: the prediction of (i) half-life of chemicals under given environmental conditions and of (ii) nanoparticle transport behavior from physicochemical properties. For that purpose, we will reconstruct previous efforts using complex workflows and architectures and simplify the models while maintaining their prediction performance. In both cases, the overall problem (predicting the fate of a

compound depending on its properties and external conditions) is modeled as a cascaded prediction model, where the prediction of one model is, with particular attention to validity and performance, entering another model as input. The approach performs well on the half-life data, while the nanoparticle data are too noisy and incomplete to warrant more than the most basic models. Overall, the reconstruction of the two applications within OpenRiskNet provides more evidence for the power and versatility of the framework.

LOGISTICS

Website and registration: <https://openrisknet.org/events/74/>

Contact: openrisknet@edelweissconnect.com

Venue

Vrije Universiteit, Auditorium, O|2 Human Life Sciences building, De Boelelaan 1108, 1081 HZ Amsterdam, The Netherlands

<https://goo.gl/maps/eoeYMjUStZqGEX437>

Recommended hotels

- Novotel Amsterdam City
<https://www.accorhotels.com/gb/hotel-0515-novotel-amsterdam-city/index.shtml>
- Motel One Amsterdam
<https://www.motel-one.com/en/hotels/amsterdam/hotel-amsterdam/>
- Amsterdam Forest Hotel <https://www.amsterdamforesthôtel.com/>
- Spa Sport Hotel Zuiver <https://zuiveramsterdam.nl/hotel>
- Olympic Hotel <http://olympic-hotel.hoteleamsterdam.net/en/>
- Ammonite Hotel Amsterdam <https://www.ammonite-hotel.com/en/index.html>



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/>



Publishing Date	Title	Authors	Category	DOI	Link
2017-01-24	OpenRiskNet Kicked off	Thomas Exner	Public communication		http://douglasconnect.com/blog/openrisknet-kicked
2017-04-04	Introduction to OpenRiskNet	Lucian Farcas	Public communication		http://www.nanosafetycluster.eu/uploads/files/NSC_Newsletter/NanoSafety_Cluster_Newsletter_Issue_9_Spring_2017.pdf
2017-04-17	Semantic prioritization of novel causative genomic variants	Imane Boudelloua, Rozaimi B. Mahamad Razali, Maxat Kulmanov, Yasmeen Hashish, Vladimir B. Bajic, Eva Goncalves-Serra, Nadia Schoenmakers, Georgios V. Gkoutos, Paul N. Schofield, Robert Hoehndorf	Peer-reviewed publication	10.1371/journal.pcbi.1005500	https://journals.plos.org/ploscompbiol/article?id=10.1371/journal.pcbi.1005500
2017-08-09	Horizon 2020 Research Success Story OpenRiskNet		Public communication		https://youtu.be/-40OGH07PaQ
2017-08-09	A global harmonized basis for testing chemical safety	Barry Hardy	Public communication		https://www.euresearch.ch/fileadmin/redacteur/Media/OpenRiskNet_Success_Story_201708_high.pdf
2017-11-02	OpenRiskNet case studies to support data and tools integration from NanoSafety Cluster	Lucian Farcas	Public communication		http://www.nanosafetycluster.eu/uploads/files/NSC_Newsletter/NSC_Autumn2017_Bulletin.pdf
2017-11-23	Integration and interoperability (conference session)	Chris Evelo, Marvin Martens, Thomas Exner, Herve Menager, Jildau Bouwman, Alessia Bardi	Presentation		http://www.opentox.net/events/opentox-euro-2017/s4
2017-12-08	OpenRiskNet reveals concepts of harmonised APIs and semantic interoperability, provides first training units, and launches Associate Partner Program	Thomas Exner	Public communication		https://openrisknet.org/news/2/
2018-01-17	The OpenRiskNet Approach towards a Semantic Interoperability Layer - Part One: Problem Definition for Datasets	Thomas Exner, Chris Evelo, Egon Willighagen, Marc Jacobs, Philip Doganis, Haralambos Sarimveis, Iseult Lynch, Stefan Kramer, Cedric Notredame, Danyel Jennen, Georgios Gkoutos, Ola Spjuth, Paul Jennings, Tim Dudgeon, Frederic Bois, Barry Hardy	Public communication		https://openrisknet.org/news/1/

Publishing Date	Title	Authors	Category	DOI	Link
2018-03-12	OpenRiskNet, an open e-infrastructure to support data sharing, knowledge integration and in silico analysis and modelling in risk assessment	Exner T, Dokler J, Bachler D, Farcial 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	Poster	10.5281/zenodo.1199287	https://zenodo.org/record/1199287#.W8CxFWgzaUk
2018-03-28	Adding ontology terms	Egon Willighagen	Tutorial		https://enanomapper.github.io/tutorials/Added%20ontology%20terms/README.html
2018-04-03	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	Peer-reviewed publication	10.1186/s13321-018-0271-1	https://jcheminf.biomedcentral.com/articles/10.1186/s13321-018-0271-1
2018-05-08	Browsing the eNM ontology with BioPortal, AberOWL and Protégé	Linda Rieswijk, Friederike Ehrhart, Egon Willighagen	Tutorial		https://enanomapper.github.io/tutorials/BrowseOntology/readme.html
2018-07-26	Big Data in Toxicogenomics: Towards FAIR predictions	Danyel Jennen	Presentation		https://drive.google.com/file/d/1amQ4yqYavW8lQp8_hbPeJMFZsaOd1qgr/view?usp=sharing
2018-08-01	OpenRiskNet flyer		Public communication		
2018-09-07	Introducing WikiPathways to support Adverse Outcome Pathways for regulatory risk assessment	Marvin Martens, Tim Verbruggen, Penny Nymark, Roland Grafström, Lyle Burgoon, Hristo Aladjov, Fernando Torres Andón, Chris T Evelo, Egon Willighagen	Poster	10.6084/m9.figshare.7038800.v1	https://doi.org/10.1016/j.toxlet.2018.06.962
2018-09-09	Entering and analysing nano safety data	Nina Jeliaskova, Egon Willighagen	Tutorial		https://enanomapper.github.io/tutorials/Entering_and_analysing_nano_safety_data/readme.html
2018-09-12	Meta-analysis for genotoxicity prediction using data from multiple human in vitro cell models	Jumamurat R. Bayjanov Jos Kleinjans Danyel Jennen	Poster	10.1016/j.toxlet.2018.06.608	
2018-09-12	OpenRiskNet roll-up banner		Public communication		
2018-09-13	Workflow: Access TG-GATEs data for selected compounds, select differentially expressed genes and identifier relevant pathways	Thomas Exner	Tutorial		https://github.com/OpenRiskNet/notebooks/blob/master/BridgeDb/DataCure%2BAOPlink.ipynb
2018-10-09	Biokinetics Modelling: use, form, inputs and outputs of PBPK models	Harry Sarimveis, Aris Dokoumetzidis, Pantelis Karatzas, Philip Doganis, Periklis Tsiros, Nikolas-Marios Katritsis, Georgia Tsiliki	Tutorial		https://drive.google.com/drive/u/0/folders/1oDP-6oTyxR0AirTIZpTQw9X1xpp32JWk

Publishing Date	Title	Authors	Category	DOI	Link
2018-10-09	OpenRiskNet e-infrastructure available to end-users	Lucian Farcas	Public communication		https://www.nanocommons.eu/wp-content/uploads/NSC%20Newsletters/NSC_Newsletter_Autumn2018.pdf?t=1539153194
2018-10-10	OpenRiskNet, an open e-infrastructure to support data sharing, knowledge integration and in silico analysis and modelling in risk assessment	Thomas Exner, Joh Dokler, Daniel Bachler, Lucian Farcas, Chris Evelo, Egon Willighagen, Danyel Jennen, Marc Jacobs, Philip Doganis, Haralambos Sarimveis, Iseult Lynch, Georgios Gkoutos, Stefan Kramer, Cedric Notredame, Ola Spjuth, Paul Jennings, Tim Dudgeon, Frederic Bois, Barry Hardy	Poster	10.1016/j.toxlet.2018.06.617	https://www.sciencedirect.com/science/article/pii/S0378427418308567?via%3Dihub
2018-10-11	Building risk assessment workflows with OpenRiskNet	Philip Doganis, Thomas Exner	Tutorial		https://docs.google.com/document/d/11GXe5gIj7q739_WCaI5v_BDugxynRGrZUu4xgIVTq6c/edit
2018-10-15	Model RX OpenRiskNet - Case study using Jaqpot web modelling platform	Philip Doganis	Tutorial		
2018-10-15	RevK Pharmacokinetics OpenRiskNet Case study using Jaqpot web modelling platform	Philip Doganis	Tutorial		https://youtu.be/AU1OEFMs3QU
2018-10-30	Tutorials OpenRiskNet public website		Tutorial		
2018-10-31	Introduction to OpenRiskNet project		Webinar recording		https://youtu.be/-SlodSpyOjl
2018-11-01	Introduction to OpenRiskNet e-infrastructure		Webinar recording		https://youtu.be/Un91N-q9BkQ
2018-11-02	Introduction to OpenRiskNet e-infrastructure	Tim Dudgeon	Presentation		https://openrisknet.org/news/14/
2018-11-02	OpenRiskNet Case Studies	Thomas Exner	Presentation		https://openrisknet.org/e-infrastructure/development/case-studies/
2018-11-02	Implementation Challenge and Associated Partner Programme	Thomas Exner	Presentation		
2018-11-02	Introduction to OpenRiskNet	Thomas Exner	Presentation		https://openrisknet.org/news/14/
2018-11-06	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	Peer-reviewed publication	10.3389/fphar.2018.01256	https://www.frontiersin.org/articles/10.3389/fphar.2018.01256/full
2018-11-06	OpenRiskNet case studies and the implementation challenge explained		Webinar recording		https://youtu.be/CNKouqvOwks

Publishing Date	Title	Authors	Category	DOI	Link
2018-11-07	Dissemination & Training Activities - Intermediate Report (Deliverable 3.4)	Doganis, Philip; Karatzas, Pantelis; Sarimveis, Harry; Dudgeon, Tim; Spjuth, Ola; Farcac, Lucian; Exner, Thomas; Lynch, Iseult; Hardy, Barry	Report	10.5281/zenodo.1479649	https://doi.org/10.5281/zenodo.1479649
2018-11-07	Report on deployment of virtual infrastructures with service discovery and container orchestration (Deliverable 2.3)	Spjuth, Ola; Dudgeon, Tim; Bachler, Daniel; Gebele, Denis; Rautenberg, Micha; Alvarsson, Jonathan; Karatzas, Pantelis; Willighagen, Egon; Evelo, Chris; Martens, Marvin; Exner, Thomas	Report	10.5281/zenodo.1479475	https://doi.org/10.5281/zenodo.1479475
2018-11-07	Initial API version provided to providers of services (Deliverable 2.2)	Rautenberg, Micha; Karwath, Andreas; Kramer, Stefan; Dudgeon, Tim; Spjuth, Ola; Bachler, Daniel; Exner, Thomas; Dokler, Joh; Sarimveis, Haralambos; Valsamis, Angelos; Doganis, Philip; Willighagen, Egon; Bois, Frederic	Report	10.5281/zenodo.1479444	https://doi.org/10.5281/zenodo.1479444
2018-11-07	Development infrastructure online (Deliverable D2.1)	Dudgeon, Tim; Spjuth, Ola; Bois, Frederic; Bachler, Daniel	Report	10.5281/zenodo.1479139	https://doi.org/10.5281/zenodo.1479139
2018-11-07	Final definition of case studies (Deliverable 1.3)	Jennings, Paul; Exner, Thomas; Farcac, Lucian; Oki, Noffisat; Sarimveis, Harry; Doganis, Philip; Jennen, Danyel; Geerke, Daan; Willighagen, Egon; Bois, Frederic; Rautenberg, Micha; Dudgeon, Tim; Hardy, Barry	Report	10.5281/zenodo.1479127	https://doi.org/10.5281/zenodo.1479127
2018-11-09	OpenriskNet webinar: demonstration on services (Nano WG - Part 2)		Webinar recording		https://youtu.be/gSDIC-pFd_8
2018-11-09	OpenRiskNet webinar: introduction, case studies and demo (Nano WG - Part 1)		Webinar recording		https://youtu.be/weOt85A_FuM
2018-11-12	First report on the management process (Deliverable 5.1)	Farcac, Lucian; Exner, Thomas; Hardy, Barry	Report	10.5281/zenodo.1484359	https://doi.org/10.5281/zenodo.1484359
2018-11-12	Report on Re-Identification Risks and Private by Design Risk Management (Deliverable 4.4)	Farcac, Lucian; Exner, Thomas	Report	10.5281/zenodo.1484320	https://doi.org/10.5281/zenodo.1484320

Publishing Date	Title	Authors	Category	DOI	Link
2018-11-12	Report of the Service Integration with OpenRiskNet - Initial Deployment (Deliverable 4.1)	Jennen, Danyel; Dudgeon, Tim; Sarimveis, Haralambos; Doganis, Philip; Karatzas, Pantelis; Rautenberg, Micha; Willighagen, Egon; Exner, Thomas	Report	10.5281/zenodo.1484309	https://doi.org/10.5281/zenodo.1484309
2018-11-12	First documentation of the core e-infrastructure (Deliverable 3.2)	Dudgeon, Tim; Christie, Alan; Bachler, Daniel; Farcas, Lucian; Sarimveis, Harry; Doganis, Philip; Karatzas, Pantelis; Spjuth, Ola; Lynch, Iseult; Hardy, Barry	Report	10.5281/zenodo.1483397	https://doi.org/10.5281/zenodo.1483397
2018-12-04	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	Peer-reviewed publication		https://www.frontiersin.org/articles/10.3389/fgene.2018.00661/
2018-12-11	OpenRiskNet factsheet		Public communication		
2018-12-13	WP4 Service Integration		Presentation		
2018-12-13	WP3 Training, Support, Dissemination		Presentation		
2018-12-13	WP2 Interoperability, Deployment and Security		Presentation		
2018-12-13	WP1 Requirement Analysis, Outreach and Case Studies		Presentation		
2019-02-06	Fully functional support infrastructure (Deliverable 3.3)		Report	10.5281/zenodo.2558122	
2019-02-06	Initial version of data management plan (Deliverable 3.1)		Report	10.5281/zenodo.2558117	
2019-02-06	Associated partner program is established (Deliverable 1.2)		Report	10.5281/zenodo.2557742	
2019-02-06	Report on requirements analysis and recommendations for WP2-4 (Deliverable 1.1)		Report	10.5281/zenodo.2557732	
2019-02-19	Expanding Adverse Outcome Pathway knowledge by creating AOP-Wiki RDF with semantic annotations to facilitate risk assessment of chemicals.	Marvin Martens, Chris Evelo, Egon Willighagen	Poster	10.6084/m9.figshare.7735067.v1	
2019-02-25	OpenRiskNet e-infrastructure Deployment	Alan Christie and Tim Dudgeon (Informatics Matters Ltd, UK)	Presentation		

Publishing Date	Title	Authors	Category	DOI	Link
2019-02-26	Learn how to deploy the OpenRiskNet virtual research environment	Alan Christie and Tim Dudgeon (Informatics Matters Ltd, UK)	Webinar recording		https://drive.google.com/drive/u/1/folders/1vQ4jEnYJzB-mDfhXq8r3GG6FACq2GOey
2019-03-18	Demonstration on data curation	Noffisat Oki (Edelweiss Connect GmbH, Switzerland), Danyel Jennen (Maastricht University, The Netherlands), Marc Jacobs (Fraunhofer Institute, Germany), Tim Dudgeon (Informatics Matters Ltd, UK)	Presentation		
2019-03-18	Final API available for internal and external service providers (Deliverable 2.4)		Report	10.5281/zenodo.2597061	
2019-03-18	Report of the Service Integration with OpenRiskNet (Intermediate Report) (Deliverable 4.2)		Report	10.5281/zenodo.2596999	
2019-03-26	Demonstration on data curation and creation of pre-reasoned datasets in the OpenRiskNet framework	Noffisat Oki (Edelweiss Connect GmbH, Switzerland), Danyel Jennen (Department of Toxicogenomics, Maastricht University, The Netherlands), Marc Jacobs (Fraunhofer Institute, Germany) and Tim Dudgeon (Informatics Matters Ltd, UK)	Webinar recording		
2019-03-27	AOPLink - Linking experimental data to Adverse Outcome Pathways	Marvin Martens, Egon Willighagen, Chris Evelo (Department of Bioinformatics, Maastricht University, The Netherlands)	Presentation		
2019-03-27	Identification and linking of data related to AOPWiki	Marvin Martens and Egon Willighagen (Department of Bioinformatics, Maastricht University, The Netherlands), Thomas Exner (Edelweiss Connect GmbH, Switzerland)	Webinar recording		
2019-04-04	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	Peer-reviewed publication		https://www.chemeng.ntua.gr/labs/control_lab/zipfiles/diazepam-paper_final.pdf
2019-04-08	AOP-DB: The Adverse Outcome Pathway Database	Holly Mortensen, Ph.D. (US EPA), Phillip Langley (ORAU-SSC) and Trevor Levey (ORAU-SSC)	Presentation		

Publishing Date	Title	Authors	Category	DOI	Link
2019-04-12	OpenRiskNet, an open e-infrastructure to support data sharing, knowledge integration and in silico analysis and modelling in predictive toxicology and risk assessment	Lucian Farcal, Denis Gebele, Evan Floden, Danyel Jennen, Egon Willighagen, Marvin Martens, Chris Evelo, Iseult Lynch, Philip Doganis, Haralambos Sarimveis, Marc Jacobs, Ola Spjuth, Tim Dudgeon, Frederic Bois, Daan Geerke, Thomas Exner	Poster		
2019-04-16	AOP-DB: The Adverse Outcome Pathway Database	Holly Mortensen, Ph.D. (US EPA), Phillip Langley (ORAU-SSC) and Trevor Levey (ORAU-SSC)	Webinar recording		
2019-05-09	Case Study description - Metabolism Prediction [MetaP]		Report		
2019-05-09	OpenRiskNet Case Studies report		Public communication	10.5281/zenodo.2652898	
2019-05-10	Case Study description - Reverse dosimetry and PBPK prediction [RevK]		Report		
2019-05-10	Case Study description - Data curation and creation of pre-reasoned datasets and searching [DataCure]		Report		
2019-05-13	How to describe OpenRiskNet services and their functionality by semantic annotation	Thomas Exner (EwC)	Presentation		
2019-05-15	How to describe OpenRiskNet services and their functionality by semantic annotation	Thomas Exner (Edelweiss Connect GmbH, Switzerland)	Webinar recording		
2019-05-27	Use Nextflow for toxicogenomics-based prediction	Evan Floden (Centre for Genomic Regulation)	Presentation		
2019-06-03	Use Nextflow for toxicogenomics-based prediction	Evan Floden (Centre for Genomic Regulation)	Webinar recording		
2019-06-24	Demonstration on OpenRiskNet approach on modelling for prediction or read across (ModelRX case study)	Philip Doganis and Haralambos Sarimveis (National Technical University of Athens, Greece)	Presentation		
2019-06-24	Deploying Applications to an OpenRiskNet Virtual Environment	Tim Dudgeon and Alan Christie (Informatics Matters Ltd, UK)	Presentation		
2019-06-25	Compute and data federation (Deliverable 2.5)	Evan Floden, Audald Lloret-Villas, Paolo Di Tommaso (CRG), Ola Spjuth (UU), Lucian Farcal (EwC), Tim Dudgeon (IM), Danyel Jennen (UM)	Report	10.5281/zenodo.3256306	

Publishing Date	Title	Authors	Category	DOI	Link
2019-06-25	Deploying Applications to an OpenRiskNet Virtual Environment	Tim Dudgeon and Alan Christie (Informatics Matters Ltd, UK)	Webinar recording		
2019-06-25	Demonstration on OpenRiskNet approach on modelling for prediction or read across (ModelRX case study)	Philip Doganis and Haralambos Sarimveis (National Technical University of Athens, Greece)	Webinar recording		
2019-06-28	Case Study description - Modelling for Prediction or Read Across [ModelRX]		Report		
2019-07-04	AOP-Wiki Resource Description Framework	Marvin Martens (Maastricht University)	Presentation		
2019-07-15	Connecting Adverse Outcome Pathways, knowledge and data with AOPLink workflows	Marvin Martens (Department of Bioinformatics, Maastricht University, The Netherlands)	Presentation		
2019-07-16	Connecting Adverse Outcome Pathways, knowledge and data with AOPLink workflows	Marvin Martens (Department of Bioinformatics, Maastricht University, The Netherlands)	Webinar recording		
2019-08-02	OpenRiskNet Part I: Development of an open e-infrastructure predictive toxicology and risk assessment	Thomas Exner, Lucian Farcac, 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	Poster	10.7490/f1000research.1117259.1	https://f1000research.com/posters/8-1335
2019-08-28	OpenRiskNet Part IV: WEKA Machine Learning Services for the Prediction of Half-Lives of Chemicals and Nanoparticle Transport	Stefan Kramer, Denis Gebele, Atif Raza	Poster	10.7490/f1000research.1117420.1	https://f1000research.com/posters/8-1515
2019-08-28	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 Farcac, Barry Hardy	Poster	10.7490/f1000research.1117419.1	https://f1000research.com/posters/8-1514

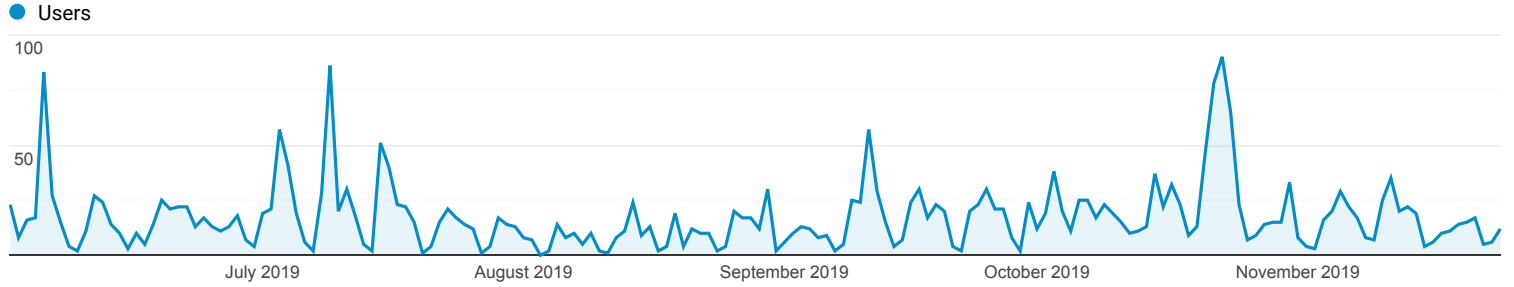
Publishing Date	Title	Authors	Category	DOI	Link
2019-08-28	OpenRiskNet Part II: Predictive Toxicology based on Adverse Outcome Pathways and Biological Pathway Analysis	Marvin Martens, Thomas Exner, Nofisat Oki, Danyel Jennen, Jumamurat Bayjanov, Chris Evelo, Tim Dudgeon, Egon Willighagen	Poster	10.7490/f1000research.1117418.1	https://f1000research.com/posters/8-1513
2019-10-07	Identification and Linking of Data related to AOPs of AOP-Wiki [AOPLink]	Marvin Martens and Egon Willighagen (Maastricht University, Department of Bioinformatics - BiGCaT)	Report		
2019-10-17	Case Study description - Toxicogenomics-based prediction and mechanism identification [TGX]	Danyel Jennen and Jumamurat Bayjanov (UM), Evan Floden (CRG)	Report		
2019-11-14	OpenRiskNet final workshop report in NanoSafety Cluster Newsletter	Lucian Farcal and Thomas Exner (EwC)	Newsletter	10.5281/zenodo.3541539	https://www.nanosafetycluster.eu/outputs/nsc-newsletter/

Audience Overview

Jun 1, 2019 - Nov 25, 2019

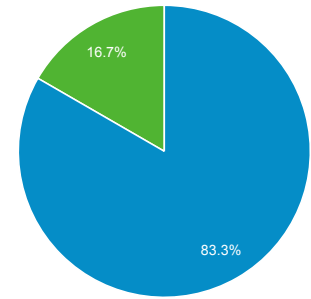
All Users
100.00% Users

Overview



Users 2,092	New Users 2,005	Sessions 3,763
Number of Sessions per User 1.80	Pageviews 10,345	Pages / Session 2.75
Avg. Session Duration 00:03:19	Bounce Rate 63.17%	

■ New Visitor ■ Returning Visitor



Country	Users	% Users
1. United States	627	28.81%
2. Netherlands	215	9.88%
3. United Kingdom	156	7.17%
4. Germany	110	5.06%
5. India	76	3.49%
6. Switzerland	74	3.40%
7. Italy	71	3.26%
8. Canada	69	3.17%
9. France	61	2.80%
10. Japan	60	2.76%

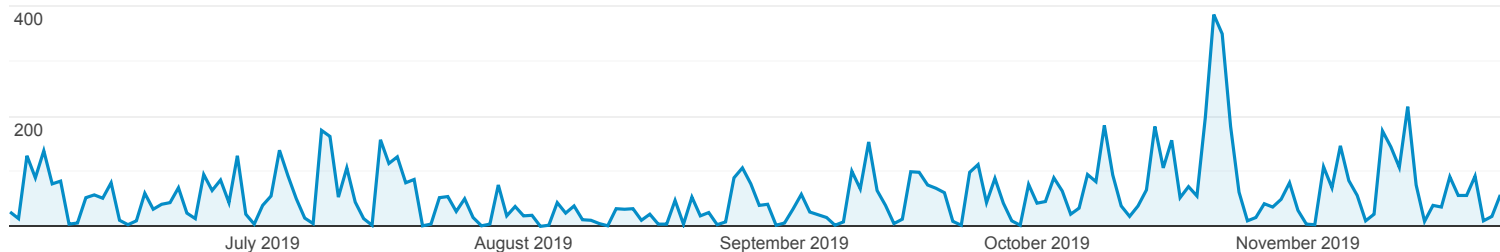
Pages

Jun 1, 2019 - Nov 25, 2019

All Users
100.00% Pageviews

Explorer

Pageviews



Page Title	Pageviews	Unique Pageviews	Avg. Time on Page	Entrances	Bounce Rate	% Exit	Page Value
	10,345 <small>% of Total: 100.00% (10,345)</small>	7,831 <small>% of Total: 100.00% (7,831)</small>	00:01:54 <small>Avg for View: 00:01:54 (0.00%)</small>	3,763 <small>% of Total: 100.00% (3,763)</small>	63.17% <small>Avg for View: 63.17% (0.00%)</small>	36.38% <small>Avg for View: 36.38% (0.00%)</small>	\$0.00 <small>% of Total: 0.00% (\$0.00)</small>
1. OpenRiskNet - Risk Assessment e-Infrastructure	1,447 <small>(13.99%)</small>	1,137 <small>(14.52%)</small>	00:01:12	1,008 <small>(26.79%)</small>	33.13%	29.37%	\$0.00 <small>(0.00%)</small>
2. Final OpenRiskNet Workshop: Creating powerful workflows combining data and software services demonstrated on risk assessment case studies • OpenRiskNet	1,294 <small>(12.51%)</small>	990 <small>(12.64%)</small>	00:05:12	726 <small>(19.29%)</small>	81.68%	65.69%	\$0.00 <small>(0.00%)</small>
3. e-Infrastructure • OpenRiskNet	1,243 <small>(12.02%)</small>	804 <small>(10.27%)</small>	00:00:55	136 <small>(3.61%)</small>	37.50%	13.60%	\$0.00 <small>(0.00%)</small>
4. Events • OpenRiskNet	911 <small>(8.81%)</small>	588 <small>(7.51%)</small>	00:00:39	110 <small>(2.92%)</small>	45.45%	10.65%	\$0.00 <small>(0.00%)</small>
5. Resources & Training • OpenRiskNet	670 <small>(6.48%)</small>	532 <small>(6.79%)</small>	00:01:58	153 <small>(4.07%)</small>	77.78%	37.91%	\$0.00 <small>(0.00%)</small>
6. Cases Studies • OpenRiskNet	332 <small>(3.21%)</small>	222 <small>(2.83%)</small>	00:01:15	56 <small>(1.49%)</small>	33.93%	16.87%	\$0.00 <small>(0.00%)</small>
7. About • OpenRiskNet	260 <small>(2.51%)</small>	212 <small>(2.71%)</small>	00:01:05	58 <small>(1.54%)</small>	89.66%	40.77%	\$0.00 <small>(0.00%)</small>
8. Lazar Toxicity Predictions • OpenRiskNet	260 <small>(2.51%)</small>	230 <small>(2.94%)</small>	00:04:02	198 <small>(5.26%)</small>	85.35%	77.69%	\$0.00 <small>(0.00%)</small>
9. News and Announcements • OpenRiskNet	257 <small>(2.48%)</small>	164 <small>(2.09%)</small>	00:01:18	18 <small>(0.48%)</small>	16.67%	12.06%	\$0.00 <small>(0.00%)</small>
10. Participate • OpenRiskNet	186 <small>(1.80%)</small>	137 <small>(1.75%)</small>	00:00:18	3 <small>(0.08%)</small>	0.00%	10.22%	\$0.00 <small>(0.00%)</small>
11. ISMB/ECCB 2019 - International Conference on Intelligent Systems for Molecular Biology & European Conference on Computational Biology • OpenRiskNet	151 <small>(1.46%)</small>	132 <small>(1.69%)</small>	00:03:38	118 <small>(3.14%)</small>	83.90%	76.16%	\$0.00 <small>(0.00%)</small>
12. Implementation challenge • OpenRiskNet	134 <small>(1.30%)</small>	116 <small>(1.48%)</small>	00:03:24	77 <small>(2.05%)</small>	84.42%	60.45%	\$0.00 <small>(0.00%)</small>
13. Connecting Adverse Outcome Pathways, knowledge and data with AOPLink workflows • OpenRiskNet	121 <small>(1.17%)</small>	107 <small>(1.37%)</small>	00:02:50	86 <small>(2.29%)</small>	86.05%	73.55%	\$0.00 <small>(0.00%)</small>
14. Demonstration on OpenRiskNet approach on modelling for prediction or read across (ModelRX case study) • OpenRiskNet	119 <small>(1.15%)</small>	100 <small>(1.28%)</small>	00:02:00	77 <small>(2.05%)</small>	77.92%	64.71%	\$0.00 <small>(0.00%)</small>
15. Services • NanoCommons	108 <small>(1.04%)</small>	64 <small>(0.82%)</small>	00:01:18	34 <small>(0.90%)</small>	55.88%	33.33%	\$0.00 <small>(0.00%)</small>
16. Case Study • OpenRiskNet	104 <small>(1.01%)</small>	76 <small>(0.97%)</small>	00:03:19	30 <small>(0.80%)</small>	53.33%	37.50%	\$0.00 <small>(0.00%)</small>
17. AOP-DB: The Adverse Outcome Pathway Database • OpenRiskNet	85 <small>(0.82%)</small>	72 <small>(0.92%)</small>	00:03:02	59 <small>(1.57%)</small>	77.97%	69.41%	\$0.00 <small>(0.00%)</small>
18. Combining neXtProt and WikiPathways strengths using SPARQL federated queries • OpenRiskNet	79 <small>(0.76%)</small>	60 <small>(0.77%)</small>	00:02:23	39 <small>(1.04%)</small>	87.18%	58.23%	\$0.00 <small>(0.00%)</small>
19. Associated Partner Programme • OpenRiskNet	76 <small>(0.73%)</small>	58 <small>(0.74%)</small>	00:02:50	12 <small>(0.32%)</small>	100.00%	40.79%	\$0.00 <small>(0.00%)</small>
20. Case Study ModelRX • OpenRiskNet	76 <small>(0.73%)</small>	54 <small>(0.69%)</small>	00:02:17	12 <small>(0.32%)</small>	33.33%	22.37%	\$0.00 <small>(0.00%)</small>

20. Case Study ModuRx • OpenRiskNet	73 (0.73%)	60 (0.69%)	00:02:47	38 (1.01%)	55.33%	22.57%	\$0.00 (0.00%)
21. Deploying Applications to an OpenRiskNet Virtual Environment • OpenRiskNet	73 (0.71%)	60 (0.77%)	00:02:36	38 (1.01%)	76.32%	57.53%	\$0.00 (0.00%)
22. Case Study DataCure • OpenRiskNet	72 (0.70%)	50 (0.64%)	00:02:57	9 (0.24%)	66.67%	25.00%	\$0.00 (0.00%)
23. Personal Data Protection and Privacy Policy • OpenRiskNet	72 (0.70%)	63 (0.80%)	00:02:49	46 (1.22%)	82.61%	63.89%	\$0.00 (0.00%)
24. Services • OpenRiskNet	64 (0.62%)	53 (0.68%)	00:05:13	5 (0.13%)	80.00%	28.12%	\$0.00 (0.00%)
25. Case Study RevK • OpenRiskNet	62 (0.60%)	53 (0.68%)	00:02:33	32 (0.85%)	81.25%	64.52%	\$0.00 (0.00%)

Rows 1 - 25 of 167

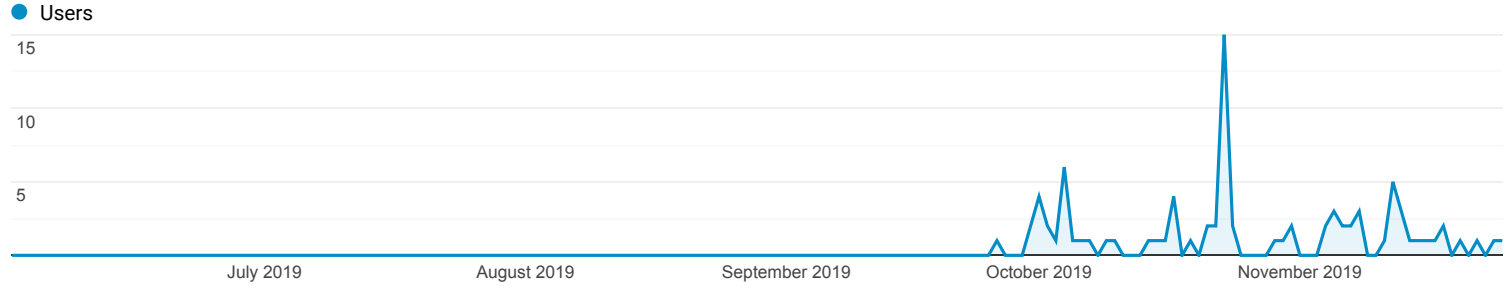


Audience Overview

All Users
100.00% Users

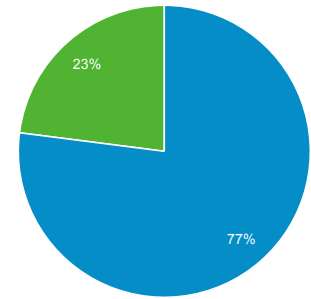
Jun 1, 2019 - Nov 25, 2019

Overview



Users 57	New Users 57	Sessions 95
Number of Sessions per User 1.67	Pageviews 182	Pages / Session 1.92
Avg. Session Duration 00:02:20	Bounce Rate 66.32%	

■ New Visitor ■ Returning Visitor



Country	Users	% Users
1. Netherlands	24	39.34%
2. United Kingdom	8	13.11%
3. Germany	7	11.48%
4. Romania	3	4.92%
5. Sweden	3	4.92%
6. Switzerland	2	3.28%
7. Greece	2	3.28%
8. Japan	2	3.28%
9. United States	2	3.28%
10. Austria	1	1.64%



eInfra Central

Benchmarking Report
on Service Catalogue Maturity for



February 2019

eInfraCentral

The mission of eInfraCentral is to *“Ensure that by 2020 a broader and more varied set of users discovers and accesses the existing and emerging Services and Resources for Research”*. The aim is to structure an open and guided discussion between e-Infrastructures to consensually define a common catalogue for their services. Based on the bottom-up consultation process, eInfraCentral designed, developed and deployed a service gateway for end-users to browse to the catalogue of services and solve the “last mile” problem.

The eInfraCentral Gateway aims at offering end-users a central entry point/gateway to a harmonized and aggregated service catalogue and an additional distribution channel to e-infrastructure services offered disparately by each e-Infrastructure or other aggregators, including service-level targets and end-user ratings.

Each of those e-Infrastructures may have their own service catalogue, perhaps with customer views and internal views, and, potentially, service portfolios. eInfraCentral intends to harmonise the parts of the service description aiming to create a homogenised customer view of the individual service catalogues and impact, to the extent possible, the deployment of full service portfolios; so, any information, which might be considered internal view to a service description, is not of direct interest to eInfraCentral.

Crucial in achieving the eInfraCentral goal is, among others, a) describing and b) exchanging service-related information to allow for increase in accessibility, discoverability, interoperability, aggregation, monitoring and comparison of services and thus their uptake and to allow for enhancing the understanding of gaps and improvements that could be delivered by e-infrastructure services. eInfraCentral, therefore, is focusing much of its efforts in those directions.

In this respect, eInfraCentral has worked in its first phase closely with the European e-Infrastructure flagship initiatives EGI, EUDAT, GÉANT, OpenAIRE and PRACE and currently also with EOSC-Hub and OpenAIRE Advance as well as 30+ other e-Infrastructure Service Providers.

From this process, eInfraCentral has devised a complete Service Description Template for an entry in a Service Portfolio in case an e-Infrastructure would like to take up and incorporate it in their Service Management Processes. In this trajectory, eInfraCentral is conducting an assessment procedure to evaluate the Service Catalogue maturity of the operating e-Infrastructures.

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Table of Contents

1. Overall Benchmarking Results	3
2. Recommendations	4
3. Comparison	7
4. Conclusions	9
5. Additional support	10

Figures

Figure 1: Overall Performance compared to Benchmark	3
Figure 2: Public Availability of Service Catalogue Indicators	7
Figure 3: Basic Service Information Indicators.....	7
Figure 4: Service Classification Indicators.....	8
Figure 5: Service Support Information Indicators.....	9
Figure 6: Service Contractual Information Indicators.....	9

Tables

Table 1: Overall Benchmarking Results.....	4
Table 2: Overall Recommendations.....	5

1. Overall Benchmarking Results

The methodology used for the benchmarking of the service providers was introduced by JNP in eInfraCentral with sole purpose to improve the “service readiness” of e-Infrastructure service providers. By taking part in the benchmarking, a service provider is awarded with a label based on 37 quality indicators assessed by three independent reviewers.

This report presents the results of the benchmarking analysis of **OpenRiskNet** based on its public website and its services descriptions in the EOSC and eInfraCentral Portals. Furthermore, a comparison to other service providers is provided and general recommendations for the service provider to improve its service catalogue and related processes.

The collected data and this benchmarking report are treated with absolute confidentiality and will not be made available to any other third party, unless the service provider has agreed beforehand in written manner. It is the sole decision of the service provider to publish the report or parts of it.

Based on the benchmarking exercise **OpenRiskNet** has gained a:

Service Catalogue Maturity Score 73%

As an overall result of the assessment, the reviewers recommend the award of the “Service Catalogue Maturity Label (Quality Label) Maturing Stage (or Silver Label)” to **OpenRiskNet**.

Table 1 on the next page presents an overview of the assessment results for the service catalogue maturity. Indicators marked “Green” reflect excellent performance while indicators marked “Yellow” indicate acceptable performance with room for improvement. Indicators marked “Red” reflect areas where significant weaknesses still exist. Lighter shades of the colours indicate the optional attributes that have a smaller effect on the Final Maturity Score.

Further improvements are seen necessary if the service provider aims to reach higher service catalogue maturity. Table 2 provides general recommendations for improvement and chapter 3 further details.

Figure 1 summarizes the performance of **OpenRiskNet** compared to the benchmark, the gold-labelled SPs (score over 80%) and the average of all SPs in the catalogue, based on a 5-pillar analysis¹: Public Availability of a Service Catalogue, Basic Service Information, Service Classification Information, Service Support Information and Service Contractual Information.

For **OpenRiskNet** to raise the service catalogue maturity assessment to a higher level, it needs to implement a number of actions as they are proposed in the following sections.

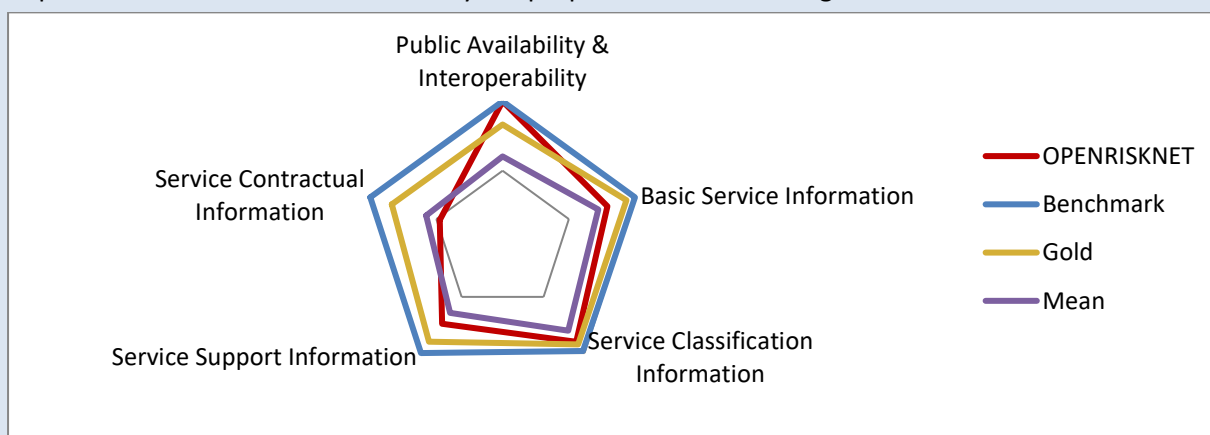


Figure 1: Overall Performance compared to Benchmark

¹ Additional pillars are currently under consideration for incorporation in the benchmarking.

Table 1: Overall Benchmarking Results

		GREEN	YELLOW	RED
M	PUBLIC AVAILABILITY	PUBLIC LINK		
		PUBLIC CATALOGUE		
		API INTEROPERABILITY		
M	BASIC SERVICE INFORMATION	Service ID		
M		Service URL		
M		Service Provider Name		
M		Service Name		
O		Service Tagline		
M		Service Description		
O		Service Options		
O		Target Users		
O		User Value		
O		User Base		
M		Service Symbol		
O		Service Multimedia		
M		SERVICE CLASSIFICATION INFORMATION	Service Version	
M	Service Last Update			
O	Service Change log			
O	Service Valid for			
M	Service Life Cycle Status			
M	Service TLR			
M	Service Category			
M	Service Subcategory			
M	Service Place			
M	Service Language			
O	Service Tags			
O	Required Services			
O	Related Services			
M	SERVICE SUPPORT INFORMATION	Service Order		
O		Service Helpdesk		
O		Service User Manual		
O		Service Training Information		
O		Service Feedback		
O	SERVICE CONTRACTUAL INFORMATION	Service Price		
M		Service Level Agreement		
O		Service Terms of Use		
O		Service Funding		

2. Recommendations

Table 2 presents an overview of the recommended improvement actions that need to be taken by **OpenRiskNet**. The recommendations focus mainly on indicators that are characterized as “Yellow” or “Red”. The order of presentation does not indicate any order of significance.

The recommendations in this document should be read and complemented with the Service Description Template (SDT) that may be downloaded from [Github](#)². The SDT offers additional recommendations and best examples of the values of all service attributes. Those recommendations are not repeated hereafter.

Table 2: Overall Recommendations

			RECOMMENDATIONS
	PUBLIC AVAILABILITY	PUBLIC LINK	
		PUBLIC CATALOGUE	
		API INTEROPERABILITY	
M	BASIC SERVICE INFORMATION	Service ID	
M		Service URL	It is recommended to rename the url of your service to match the id name, always with the shortest possible alias. e.g. https://openrisknet.org/e-infrastructure/openrisknet.jaqpot_
M		Service Provider Name	
M		Service Name	It is recommended to harmonise the names of your services/resources and update the URLs accordingly.
O		Service Tagline	It is recommended to engage marketing specialists to come up with a catch phrase that can aid service discoverability and visibility.
M		Service Description	
O		Service Options	It is recommended to review this attribute for all services/resources and provide an harmonised and clear description of the possible service instantiation options.
O		Target Users	
O		User Value	
O		User Base	It is recommended to provide a description as quantified as possible. e.g. "900+ data providers in Europe with different compatibility levels."
M		Service Symbol	
O		Service Multimedia	
M		Service Version	
M		Service Last Update	
O	Service Change log		
O	Service Valid for	It is strongly recommended to provide an expiring date for the services/resources. The expiring date should imply validity period until 23:59:59.	
M	Service Life Cycle Status		
M	Service TLR		
M	Service Category		
M	Service Subcategory		
M	Service Place		
M	Service Language		
O	Service Tags		
O	Required Services	Please review if other services/resources (Service IDs) are required to instantiate this service/resource.	
O	Related Services	It is recommended to update this attribute that may be used for cross-selling, promotion of other services/resources and engaging the user with the catalogue.	

² <https://github.com/eInfraCentral/docs>

M O O O O	SERVICE SUPPORT INFORMATION	Service Order	It is recommended to provide a link that leads to the direct ordering of each service/resource.
		Service Helpdesk	
		Service User Manual	
		Service Training Information	It is recommended to provide Training Information for all services/resources with links that direct to your website.
		Service Feedback	It is recommended to encourage feedback on your services/resources, by providing a link for feedback.
O M O O	SERVICE CONTRACTUAL INFORMATION	Service Price	It is strongly recommended to provide a link to accurate information on the pricing of the services/resources.
		Service Level Agreement	It is recommended to provide a link to the Service Level Agreement for each service/resource. Scan the catalogue for examples.
		Service Terms of Use	It is recommended to provide a link to the Terms of Use of each service/resource.
		Service Funding	

3. Comparison

3.1 Public Availability of Service Catalogue

As depicted in Figure 2, **OpenRiskNet** has a link to services in its landing page or a service catalogue in its public site. The existence of both is essential for every service providers as without them the customer cannot shape a clear an accurate view about the services provided. OpenRiskNet ranks well above the average in these two attributes. OpenRiskNet’s decision to implement the API is in the right direction.

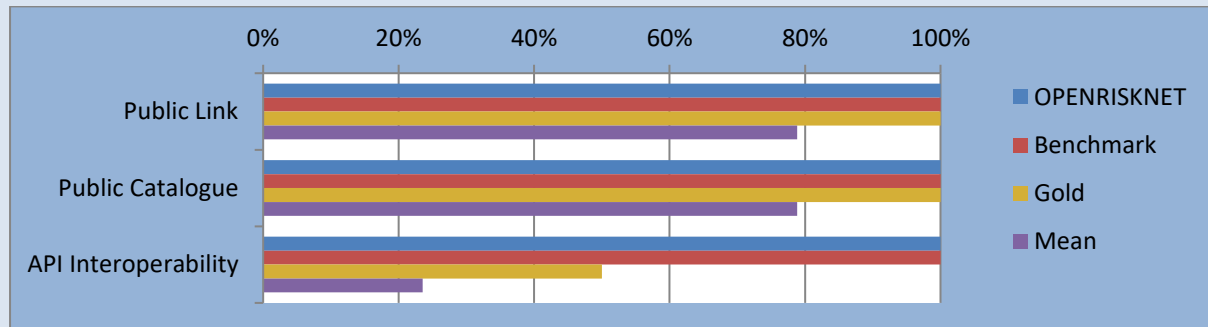


Figure 2: Public Availability of Service Catalogue Indicators

3.2 Basic Service Information

As depicted in Figure 3, **OpenRiskNet** performs “green”, scoring between 80% and 100% in **seven out of the twelve indicators** of the category Basic Service Information.

The attributes below average are: Service URL (OpenRiskNet: 70%, Mean: 78%), Name (OpenRiskNet: 70%, Mean: 88%), Tagline (OpenRiskNet: 70%, Mean: 72%), Options (OpenRiskNet: 30%, Mean: 46%) and User Base (OpenRiskNet: 30%, Mean: 44%). Due to the mandatory nature of two attributes (URL and Name), they have a considerable negative impact to the overall score.

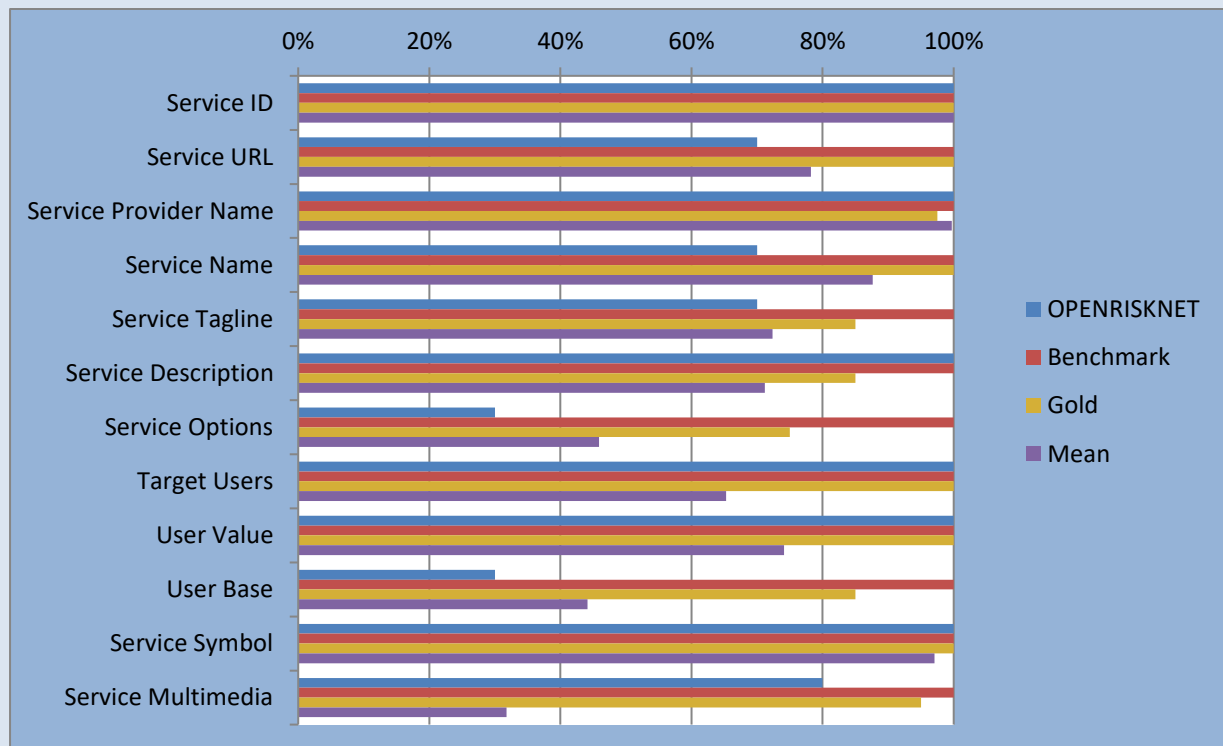


Figure 3: Basic Service Information Indicators

3.3 Service Classification Information

As depicted in Figure 4, **OpenRiskNet** performs “green”, with the maximum score of 100%, in **eleven out of the thirteen indicators** of the category Service Classification Information.

This is an impressive performance that brings OpenRiskNet at the same level as the Gold Label Average for the Basic Service Information Pillar.

Only one attribute is found to be below the average: Service Valid for. The Service Valid for should be filled with the date up to when the service is valid for.

The attribute Related Services is equal to the average at 70%. It is recommended to fill the Related Services with other services that are commonly used with this service.

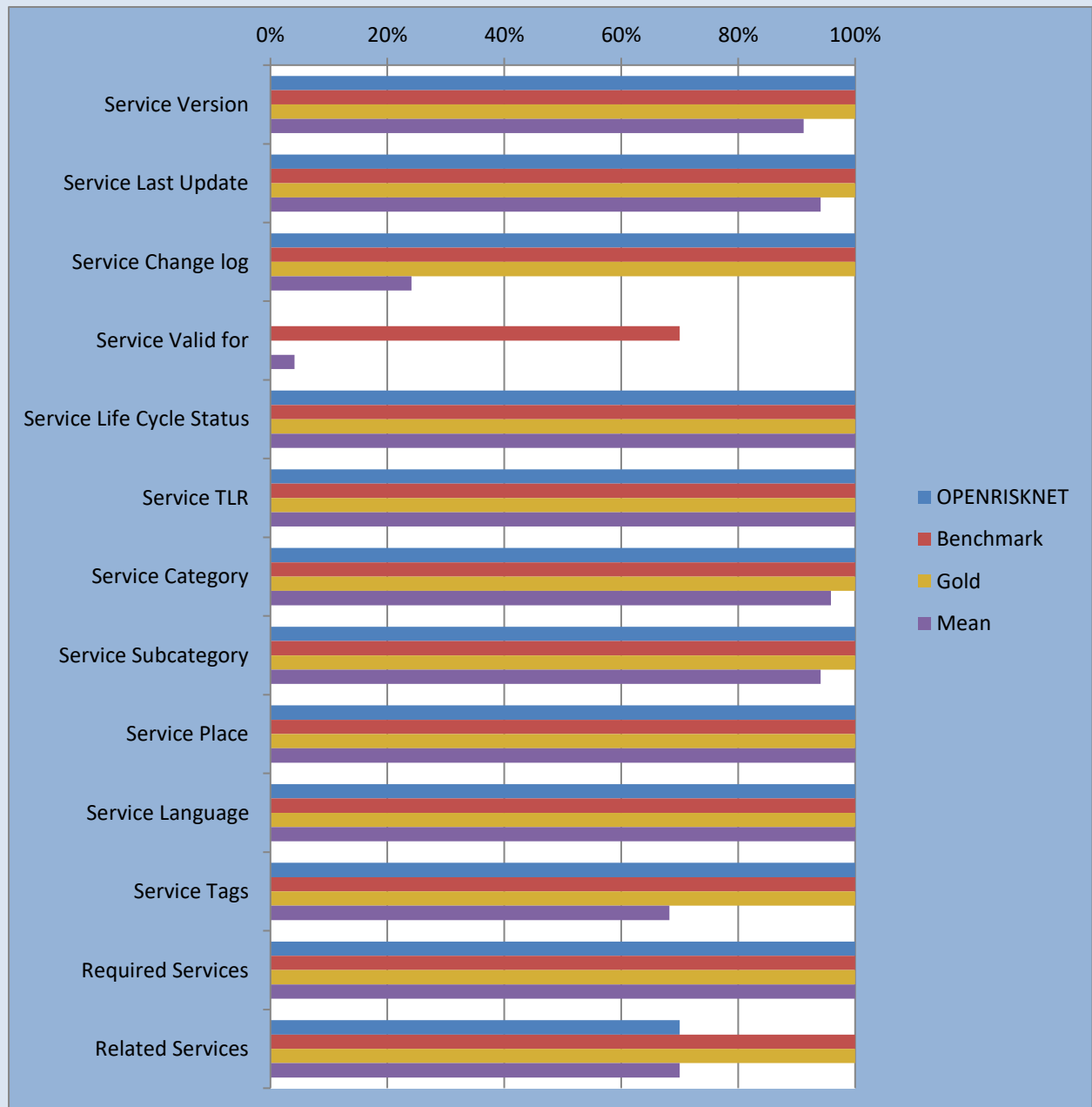


Figure 4: Service Classification Indicators

3.4 Service Support Information

As depicted in Figure 5, **OpenRiskNet** performs “green” in **two out of the five indicators** of the category Service Support Information. It should be noted that OpenRiskNet performs above the average in 4 out of 5 attributes: Service Helpdesk (OpenRiskNet: 100%, Mean: 87%), User Manual (OpenRiskNet: 100%, Mean: 64%), Training Information (OpenRiskNet: 70%, Mean 61%) and Feedback (OpenRiskNet: 50%, Mean 48%). It only performs below the average for Service Order (OpenRiskNet 50%, Mean 62%). Due to the mandatory nature of this attribute, it has a considerable negative impact to the overall score.

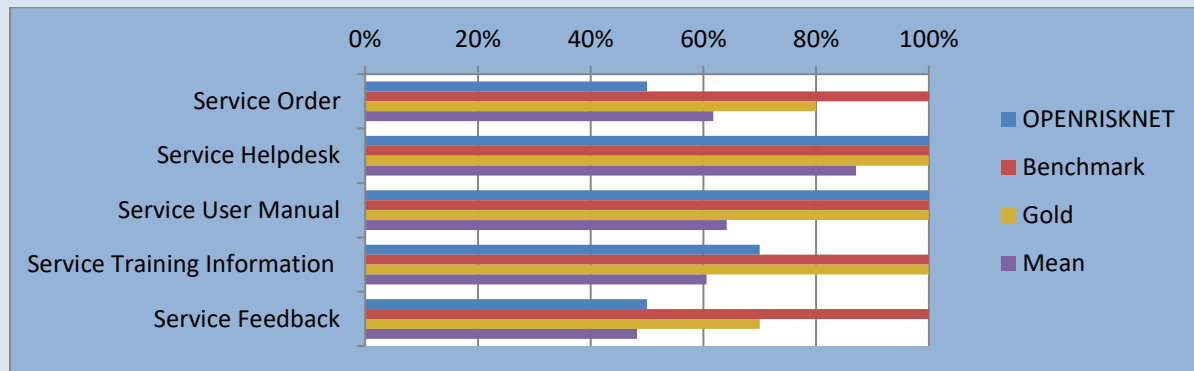


Figure 5: Service Support Information Indicators

3.5 Service Contractual Information

As depicted in Figure 6, **OpenRiskNet** performs “green”, scoring 100%, in **one out of the four indicators** of the category Service Contractual Information. OpenRiskNet performs below the average for the other 3 attributes: Service Price (OpenRiskNet: 0%, Mean: 44%), Service Level Agreement (OpenRiskNet: 40%, Mean: 55%) and Terms of Use (OpenRiskNet: 50%, Mean: 62%).

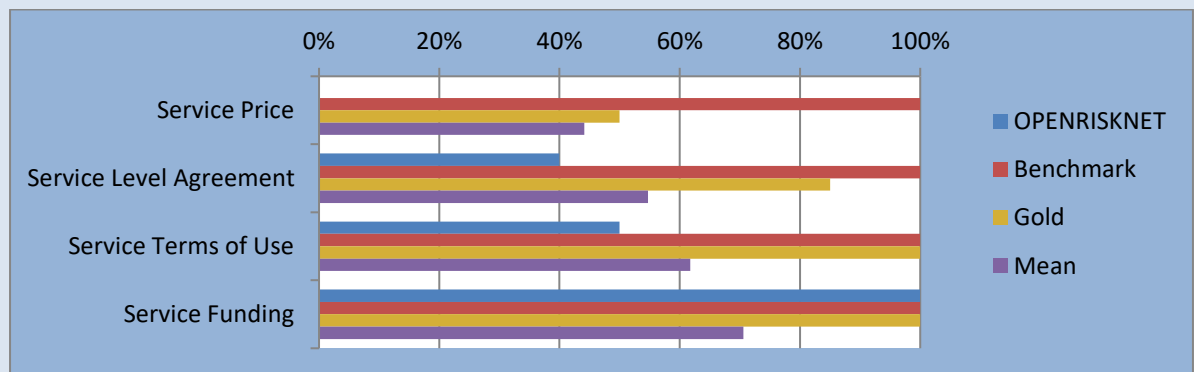


Figure 6: Service Contractual Information Indicators

4. Conclusions

Conclusively, it has been found that OpenRiskNet has an overall very good performance with maturing services. The qualitative evaluation showed that OpenRiskNet is slightly above the mean of all the Service Providers in the Catalogue. It is important to note that OpenRiskNet is around the same level with the Gold Label average for the attributes in the Service Classification Information Pillar and is significantly above it for the Public Availability & Interoperability Pillar. Finally, it lacks mostly at the Service Contractual Information Pillar, where it is found to perform below the average.

5. Additional support

Should **OpenRiskNet** require any external support for advancing its Service Catalogue Maturity and/or implementing any further Service Description improvements in this respect, JNP staff would be happy to offer its advisory expertise to aid in this direction. If so, please contact us at your convenience by email at eic@jnp.gr, nominating the appropriate representative for your organisation, and a member of our team will promptly follow up on this matter.