OpenRiskNet, an open e-infrastructure to support data sharing, knowledge integration and *in silico* analysis and modelling in predictive toxicology and risk assessment
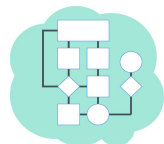
Workshop
Creating powerful workflows combining data and software services demonstrated on risk assessment case studies

OpenRiskNet
RISK ASSESSMENT E-INFRASTRUCTURE
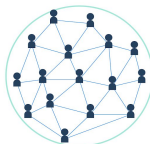
23 - 24 October 2019, Amsterdam, Netherlands | https://openrisknet.org/

How?

Easily accessible, standardised, harmonised, scalable and robust infrastructure
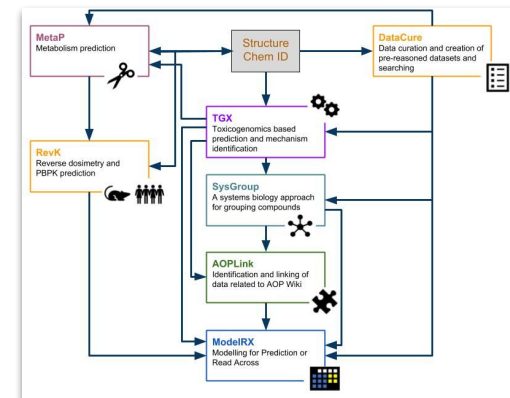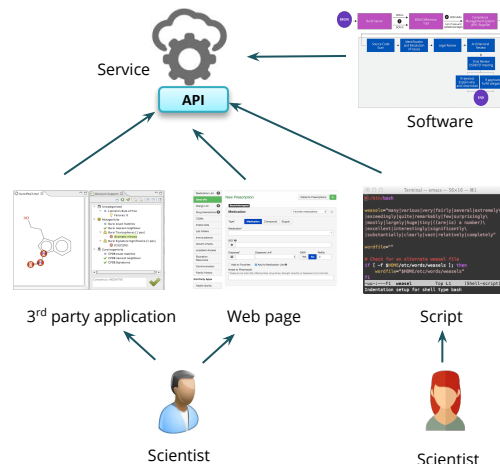
For whom?

Researchers
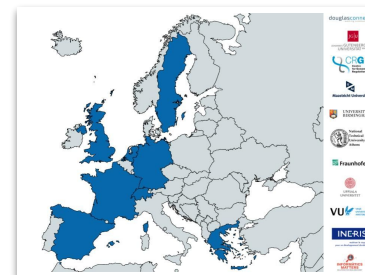Risk assessors
Regulators
Informed public

To what end?

Improvement of industrial risk assessments
Prototyping of new services and apps
Access to integrated resources
Complete and qualified system
Support for innovative product development

Service
API
Software

3rd party application
Web page
Script

Scientist
Scientist

MetaP — Metabolism prediction
Structure Chem ID
DataCure — Data curation and creation of pre-reasoned datasets and searching
RevK — Reverse dosimetry and PBPK prediction
TGX — Toxicogenomics based prediction and mechanism identification
SysGroup — A systems biology approach for grouping compounds
AOPLink — Identification and linking of data related to AOP Wiki
ModelRX — Modelling for Prediction or Read Across

E-infrastructure providing resources and services to a variety of communities requiring risk assessment, including **chemicals, cosmetic ingredients, therapeutic agents and nanomaterials**:
- **Harmonising** access to data and facilitating **interoperability** of software,
- Easily **deployable** to single computers, public and in-house cloud solutions,
- Addressing the needs of **industry and academic researchers, risk assessors and regulators.**

H2020-EINFRA Call
2016-2019 3 years project
3 mil Total funding
11 Partner Organisations
12 Associated Partners
7 Case studies

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Day 1 - 23 October 2019

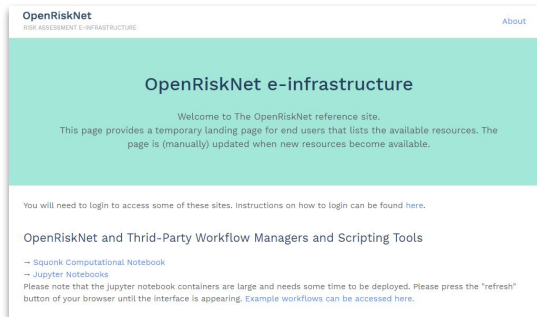| 8:30-9:00	Registration	
9:00-9:10	Welcome and introduction to the workshop	Thomas Exner (Edelweiss Connect, GmbH, Switzerland)
9:10-9:30	OpenRiskNet Case studies introduction and concept	Paul Jennings (Vrije Universiteit Amsterdam, The Netherlands)
9:30-10:30 8 min / case study	OpenRiskNet **Case studies** (flash presentations): • 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	*Coffee break (incl. posters viewing)*	
	OpenRiskNet demo & training sessions	
11:00-12:30	**Workflows**: practical example of Jupyter notebooks use, Data curation example, workflow across multiple case studies	Marvin Martens (UM) and Thomas Exner (EwC)
12:30-13:30	*Lunch break*	
13:30-15:00	Parallel sessions: • **Group 1: Deploying Applications** (addressed to developers, services providers and infrastructure admins) (Room: 12W24) • **Group 2: Modelling exercise** (built around the ModelRX case study, support of the DataCure) (addressed to end-users) (Room: 01W08)	Tim Dudgeon (IM) Philip Doganis and Pantelis Karatzas (NTUA), Denis Gebele (JGU), Tomaž Mohorič (EwC), and Jonathan Alvarsson (UU)
15:30-16:00	*Coffee break (incl. posters viewing)*	
16:00-17:30	Parallel sessions: • **Group 1: Q&A Deploying Applications** (Room: 12W24) • **Group 2: Ontology and semantic annotations** (Room: 01W08)	Tim Dudgeon (IM) Egon Willighagen (UM)
18:00-	*Dinner - Buffet organised at workshop venue*	

Workshop feedback
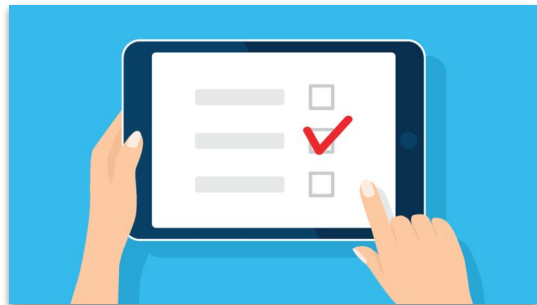
https://forms.gle/5rRuxh14CxLVoFUm9

Reference Environment

https://home.prod.openrisknet.org

www.openrisknet.org

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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 in silico 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)
12:00-12:30	**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	Iseult Lynch (University of Birmingham, UK)
14:00-15:00	1. Introduction to the **European Open Science Cloud (EOSC)** (10 min) 2. **OpenAIRE**: an EOSC implementation project (10 min)	Alessia Bardi (Institute of Science and Technology of Information, CNR, Italy)
	3. **eInfraCentral**: an EOSC implementation project (10 min)	Bjorn Backeberg (EGI Foundation, The Netherlands) on behalf of Jelena Angelis (EFIS Centre, Belgium)
	4. **EOSC-hub**: an EOSC implementation project (10 min)	Bjorn Backeberg (EGI Foundation, The Netherlands)
	5. **Technical demo** of cloud and storage services in EOSC (20 min)	Yin Chen (EGI Foundation, The Netherlands)
15:00-15:30	*Coffee break*	
15:30-16:00	Panel discussion: lesson learned and looking ahead to the next steps	
16:00-16:15	**Closing session**	