

OpenRiskNet, an open e-infrastructure to support data sharing, knowledge integration and *in silico* analysis and modelling in predictive toxicology and risk assessment

Lucian Farcas^{1*}, Denis Gebele², Evan Floden³, Danyel Jennen⁴, Egon Willighagen⁴, Marvin Martens⁴, Chris Evelo⁴, Iseult Lynch⁵, Philip Doganis⁶, Haralambos Sarimveis⁶, Marc Jacobs⁷, Ola Spjuth⁸, Tim Dudgeon⁹, Frederic Bois¹⁰, Daan Geerke¹¹, Thomas Exner¹

Introduction

OpenRiskNet is an e-infrastructure for **predictive toxicology** and chemical and nanomaterial **risk assessment**. It is

- **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

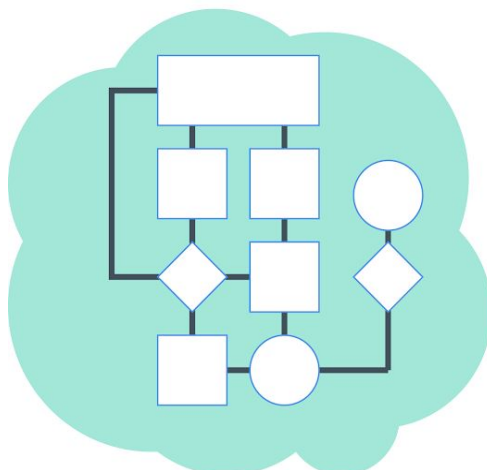
 **12** Associated Partners

 **7** Case studies

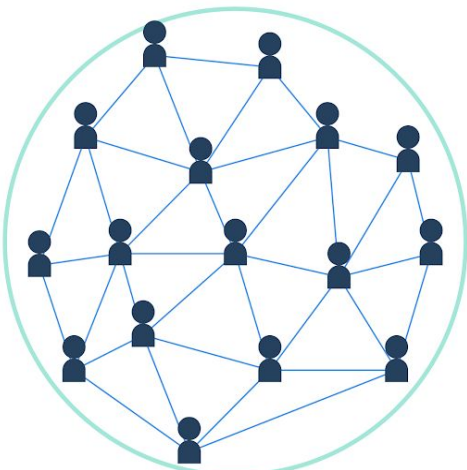
How?

For whom?

To what end?



Easily accessible, standardised, harmonised, scalable and robust infrastructure



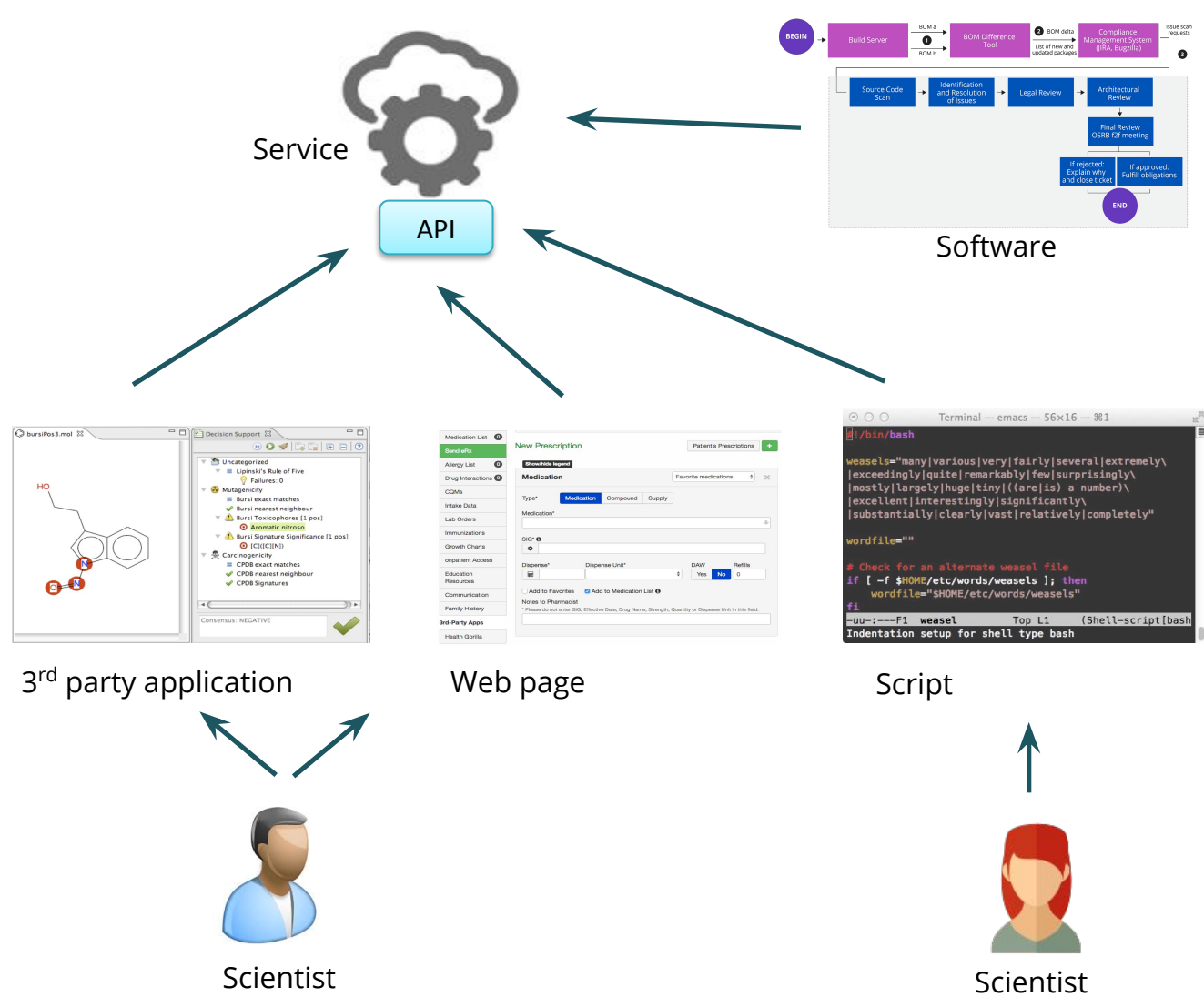
Researchers
Risk assessors
Regulators
Informed public



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

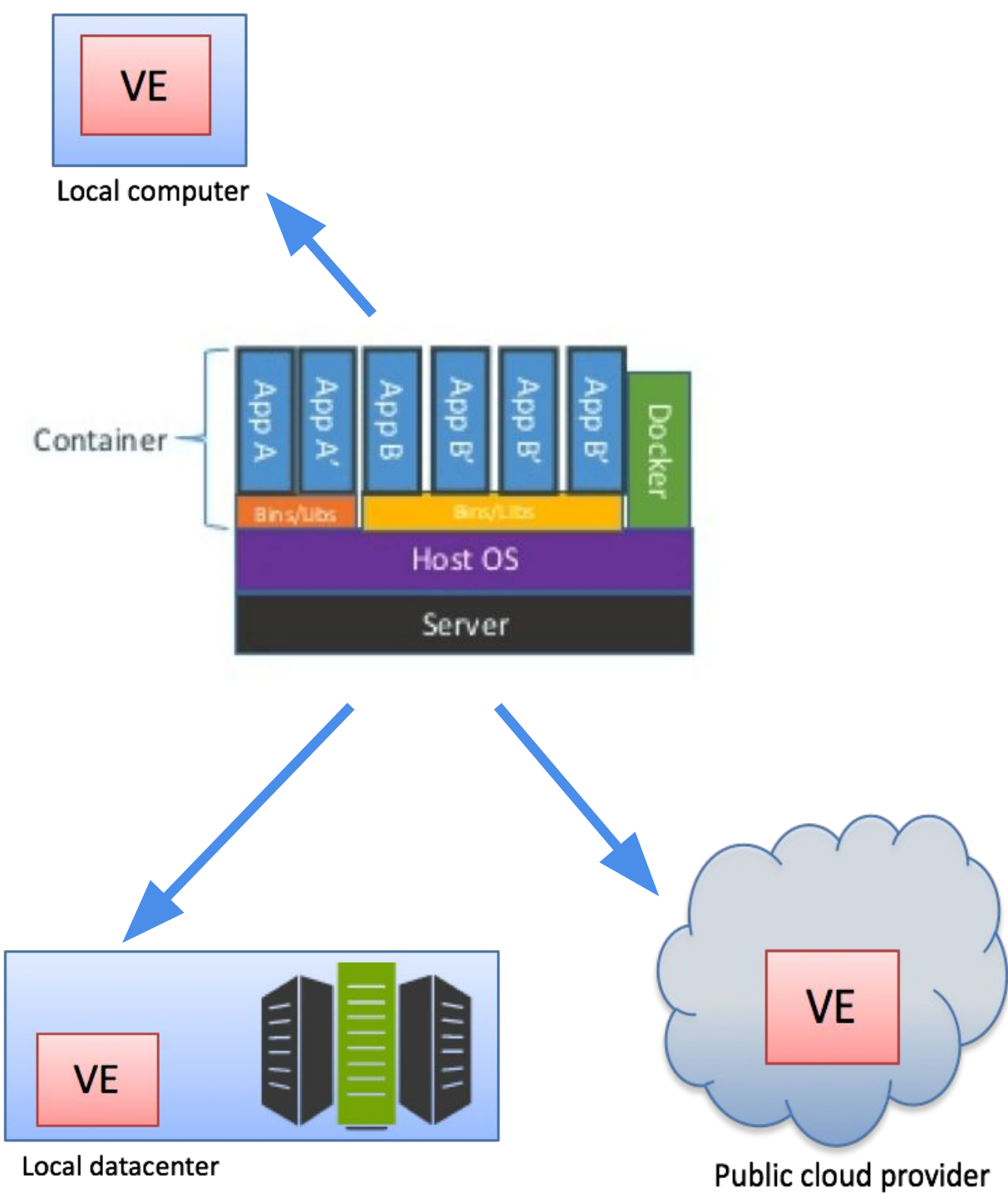
Service-oriented science, containerisation, deployment

- Uses modern and established tools and frameworks supported by broad scientific communities and industry
- Offers an agile and scalable environment to use, and a straightforward platform to extend
- Allows language-agnostic integration of diverse software
- Reduces extra work for integration
- Reduces risk and improve sustainability

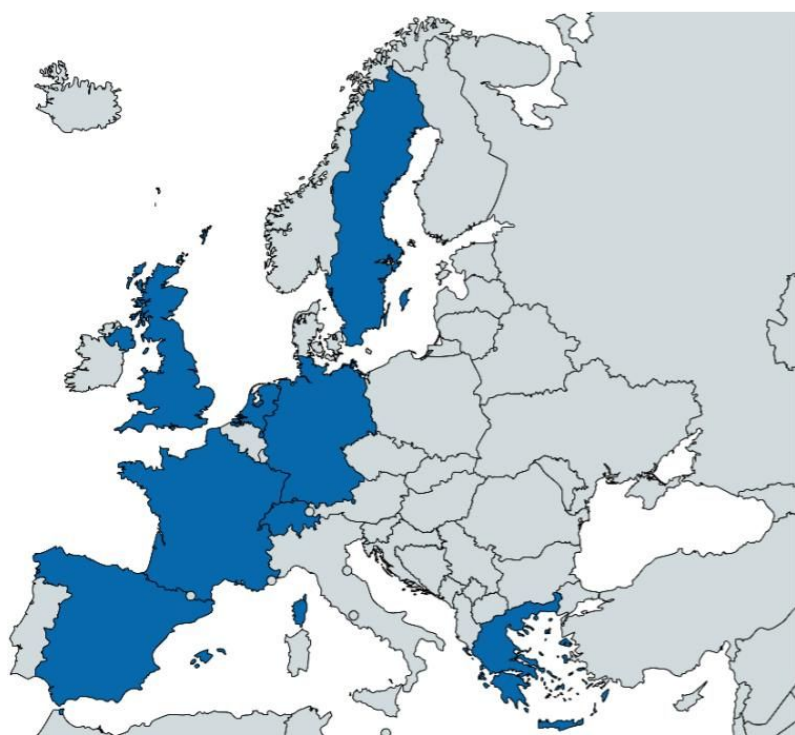


Main concepts:

1. **REST services** providing data and processing/analysis/modelling tools (by OpenRiskNet and associated partners)
2. **Harmonize APIs** in an bottom-up approach
3. Microservice architecture based on **containerization and container orchestration** accompanied by a **discovery service**
4. **Virtual environments**, which can be deployed on public or in-house clouds - reference environment available at <https://home.prod.openrisknet.org>



OpenRiskNet partners



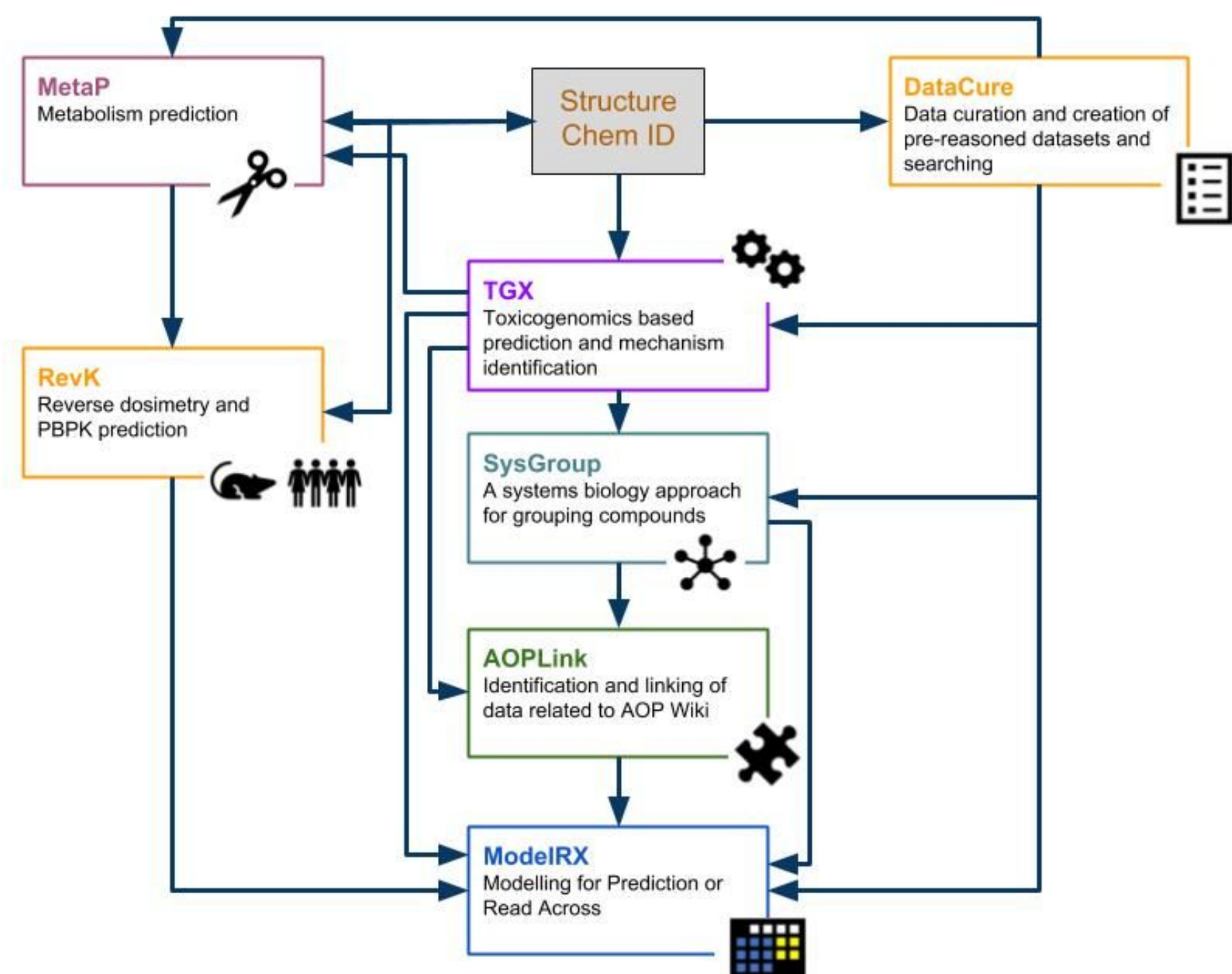
-  Edelweiss Connect
-  University of Birmingham
-  Fraunhofer
-  Vrije Universiteit Amsterdam
-  University of Athens
-  University of Mainz
-  University of Amsterdam
-  University of Edinburgh
-  University of Manchester
-  University of Liverpool
-  University of Nottingham

- ¹Edelweiss Connect GmbH, Basel, Switzerland;
- ²Johannes Gutenberg-Universitat 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.

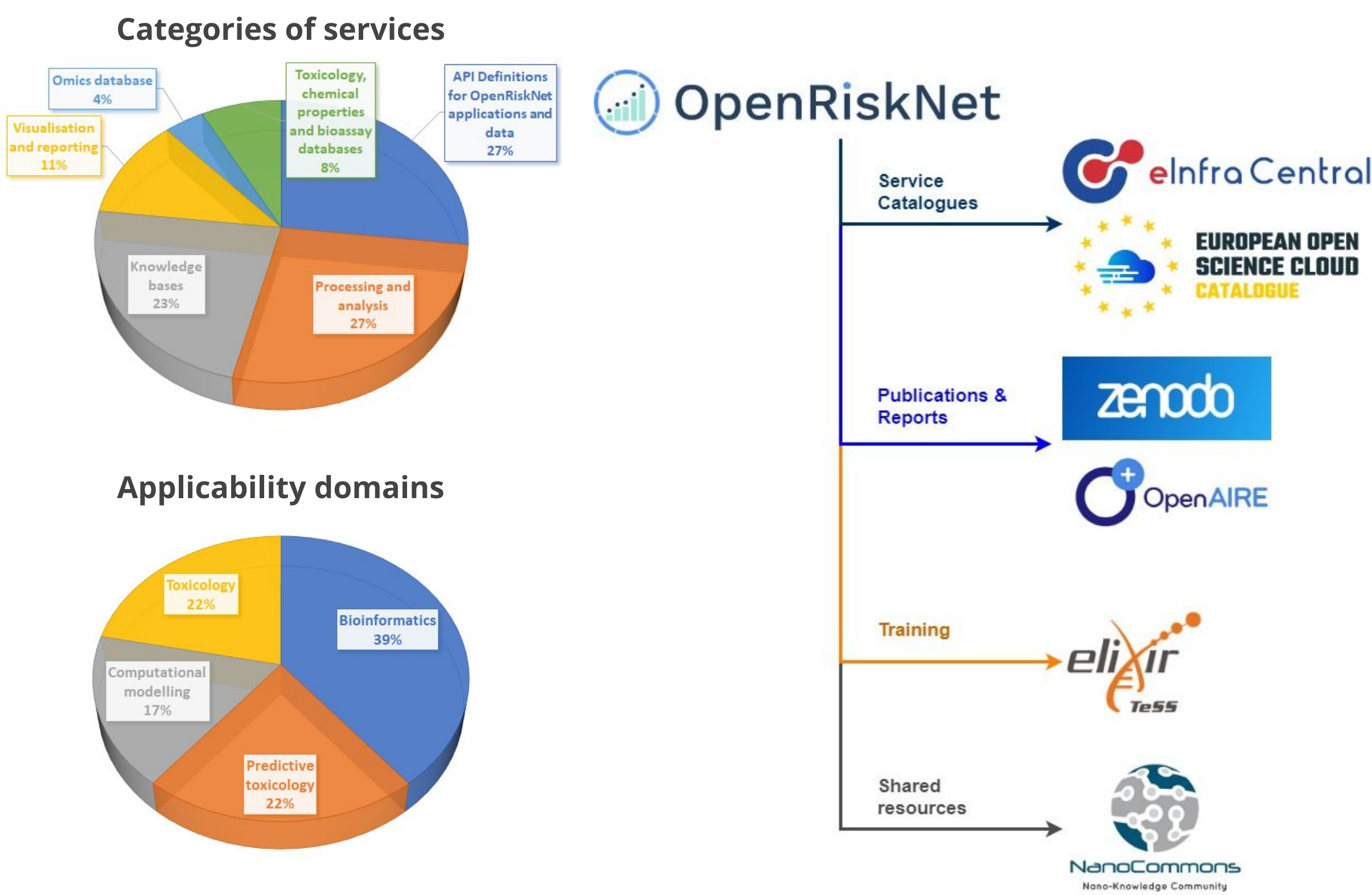
Case studies

- Case-study-driven development is used to:
- Test and evaluate the solutions provided,
 - Demonstrate the ability to satisfy stakeholder groups requirements,
 - Present real-world applications,
 - Guide the prioritisation of data sources and tools.

A workflow for the safety assessment of chemicals without animal testing developed within the SEURAT-1 project (*Berggren et al., 2017*) was selected to guide the definition of the case studies.
This workflow constructs a hypothesis based on existing data, computational modelling, biokinetic considerations, and then, targeted non-animal testing.
<https://openrisknet.org/e-infrastructure/development/case-studies/>



Services Catalogue, dissemination & sustainability



   @OpenRiskNet

Other resources

Service Catalogue <https://openrisknet.org/e-infrastructure/services/>
Publications & Training Resources <https://openrisknet.org/library/>
Conferences and Events <https://openrisknet.org/events/>

Technical Documentation <https://github.com/OpenRiskNet>

Help Desk <https://openrisknet.freshdesk.com/>
Contact openrisknet@edelweissconnect.com

Resources for end-users

Resources for developers

Acknowledgements

OpenRiskNet (Project no. 731075) is funded by the European Commission within the Horizon 2020 Programme

