OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE

douglasconnect working communities

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

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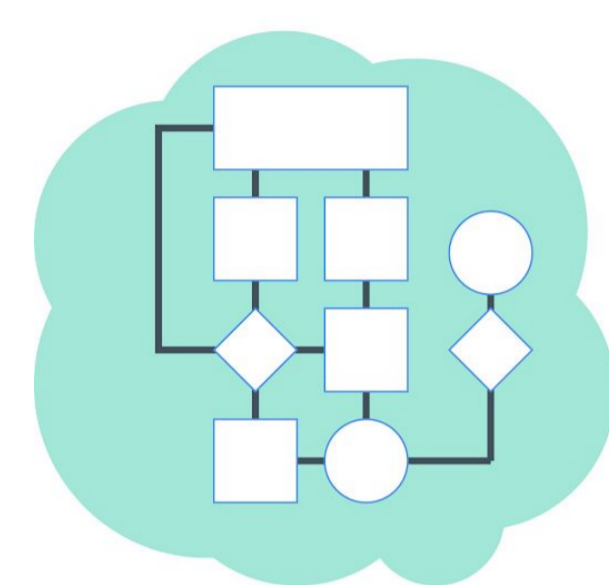Thomas Exner | thomas.exner@douglasconnect.com

Introduction

OpenRiskNet is
- a virtual research environment for **predictive toxicology** and chemical and nanomaterial **risk assessment,**
- **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, regulators and informed public.**
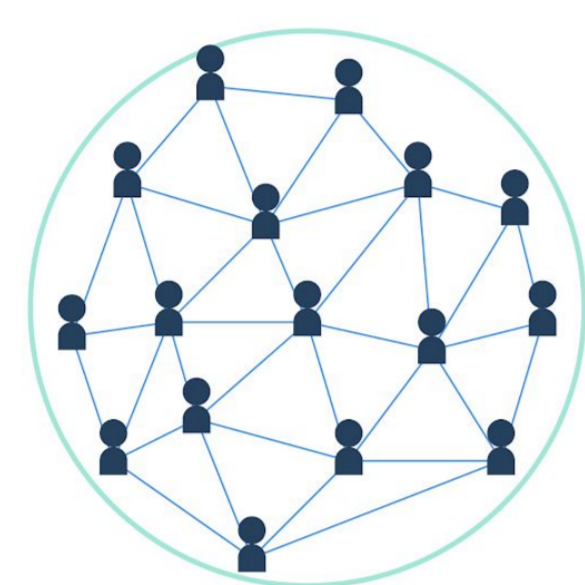

| How?	For whom?	To what end?
Easily accessible, standardised, harmonised, scalable and robust infrastructure	Researchers Risk assessors Regulators Informed public	Improvement of industrial risk assessments Prototyping of new services and apps Access to integrated resources Complete and qualified system Support for innovative product development

Service-oriented science, containerization, deployment

- Uses modern and established tools and frameworks supported by 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
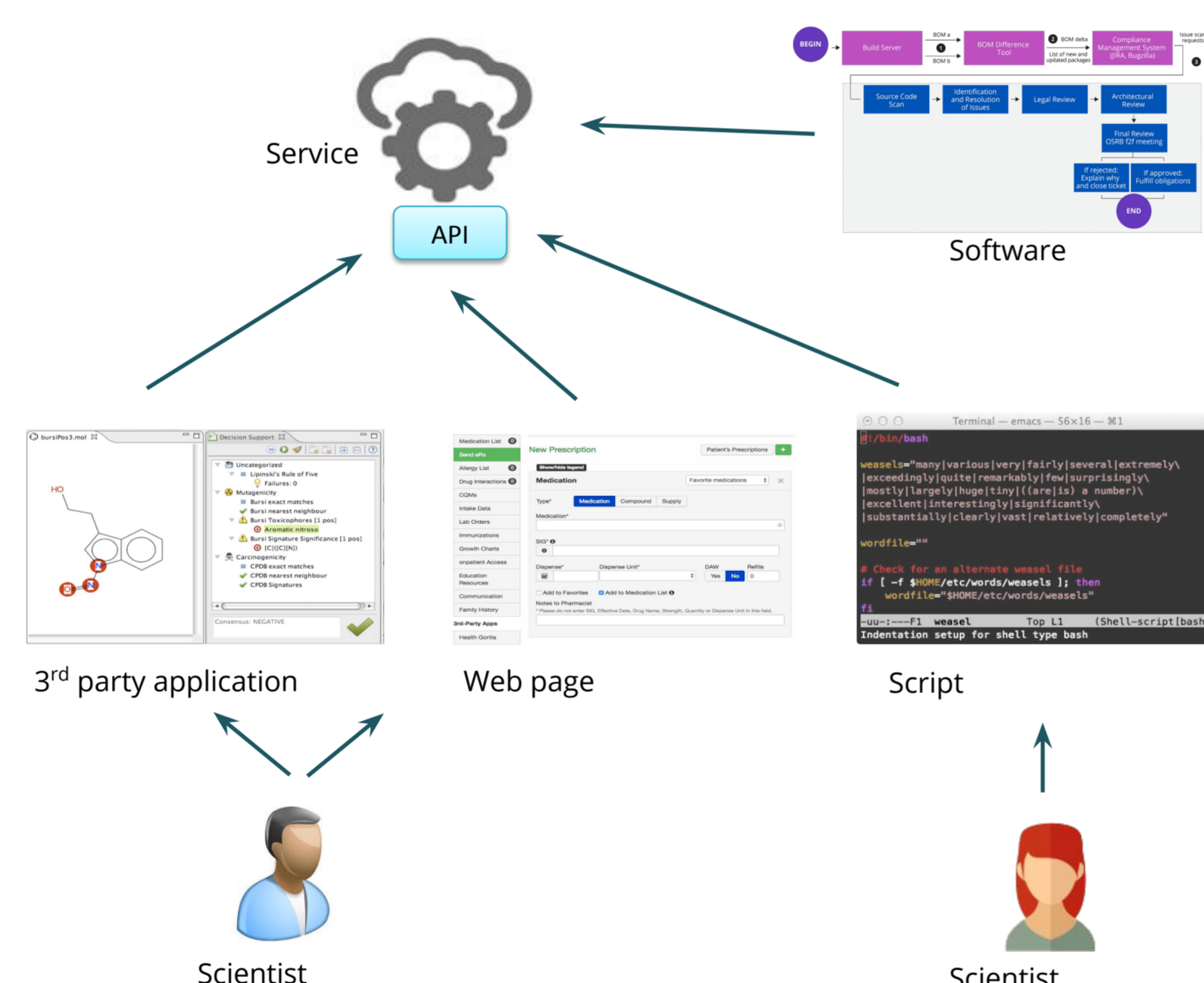
Main concepts:

1. **REST services** providing data and processing/analysis/modelling tools (provided 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 infrastructures**, which can be deployed on public or in-house clouds - reference environment available at https://home.prod.openrisknet.org
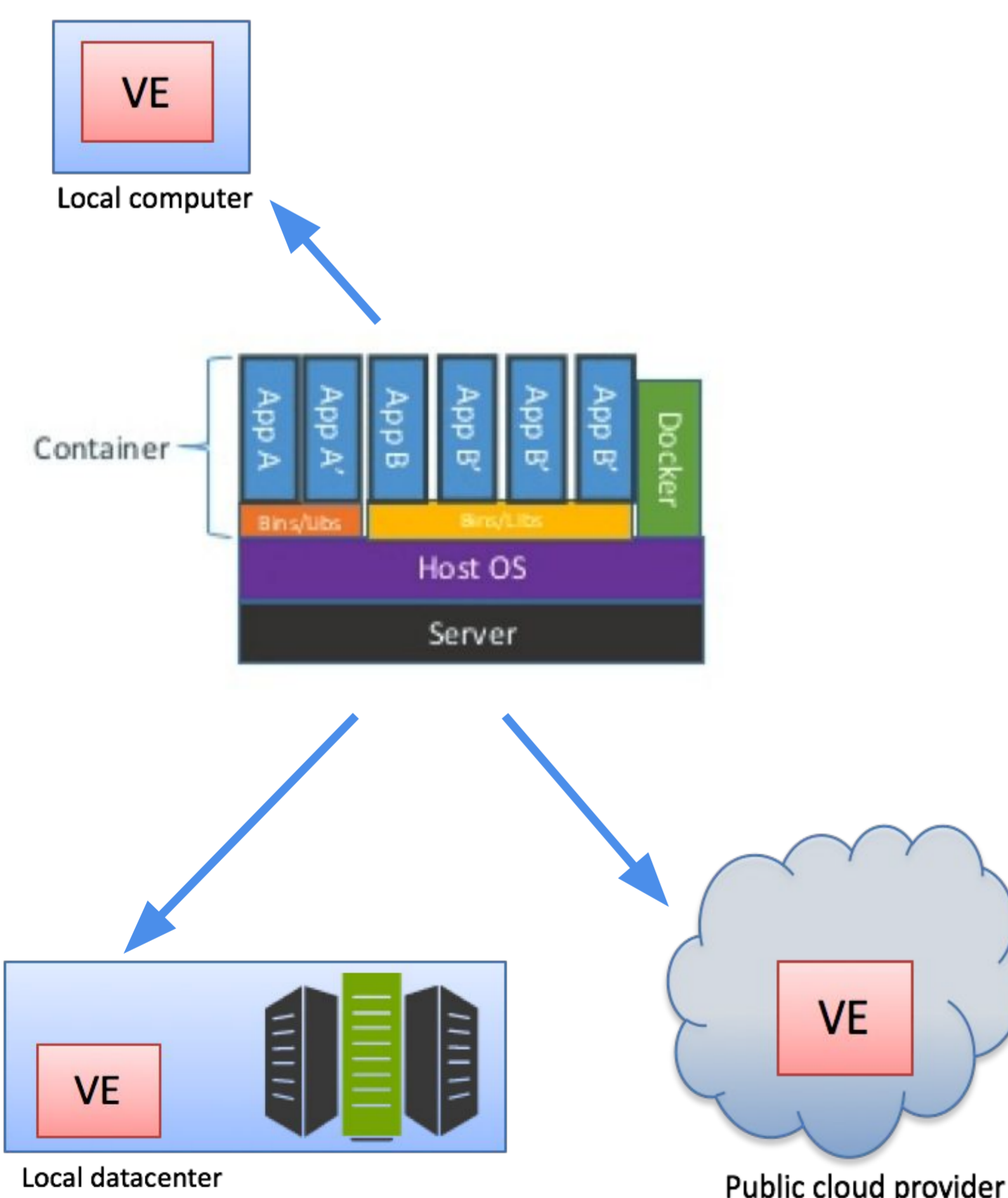
OpenRiskNet partners

P1 Douglas Connect GmbH, Switzerland (DC)
P2 Johannes Gutenberg-Universität Mainz, Germany (JGU)
P3 Fundacio Centre de Regulacio Genomica, Spain (CRG)
P4 Universiteit Maastricht, Netherlands (UM)
P5 The University Of Birmingham, United Kingdom (UoB)
P6 National Technical University Of Athens, Greece (NTUA)
P7 Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V., Germany (Fraunhofer)
P8 Uppsala Universitet, Sweden (UU)
P9 Medizinische Universität Innsbruck, Austria (MUI)
P10 Informatics Matters Limited, United Kingdom (IM)
P11 Institut National de l'Environnement et des Risques INERIS, France (INERIS)
P12 Vrije Universiteit Amsterdam, Netherlands (VU)

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 prioritization 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 7 case studies. This workflow constructs a hypothesis based on existing data, computational modelling, biokinetic considerations, and then, targeted non-animal testing.
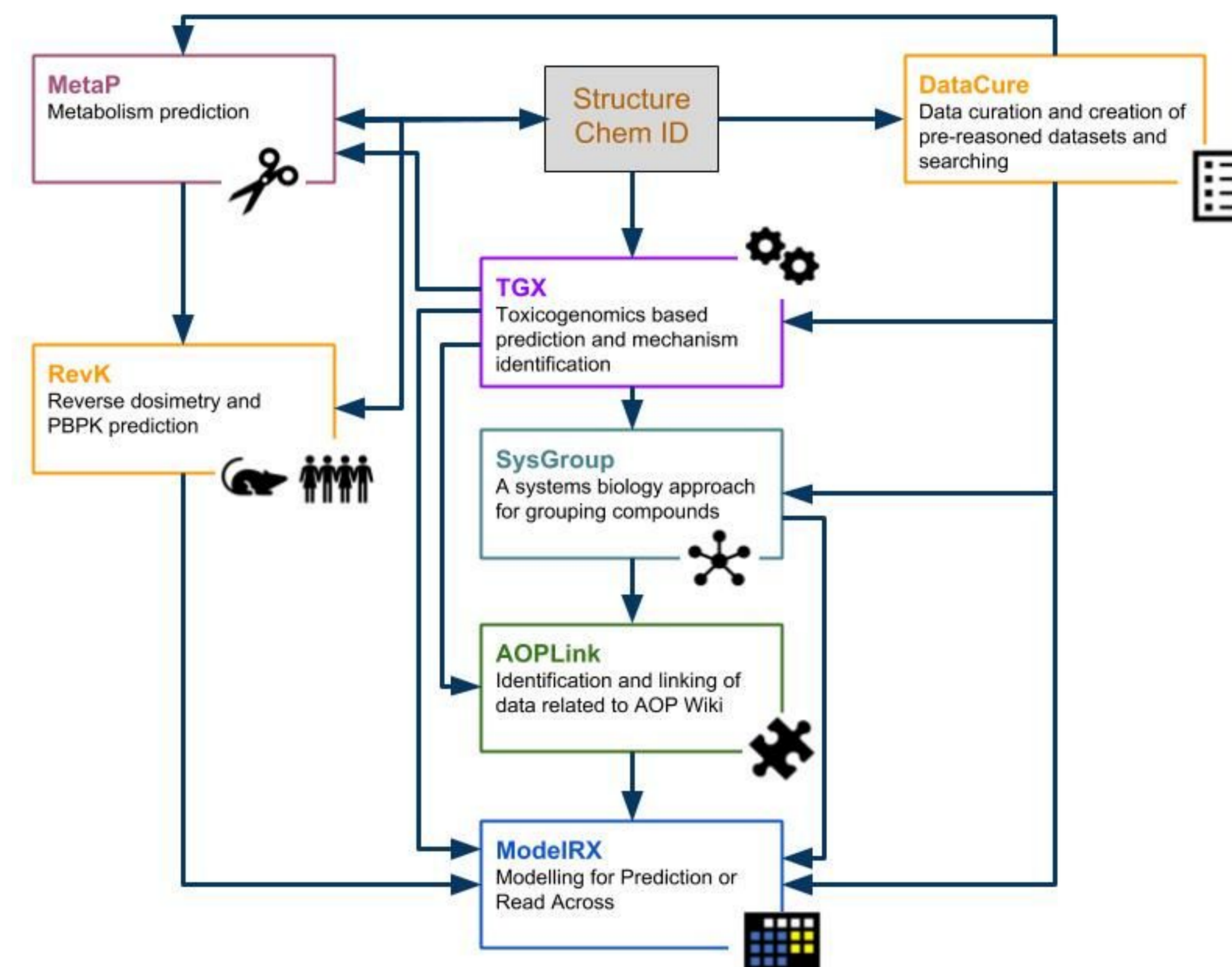
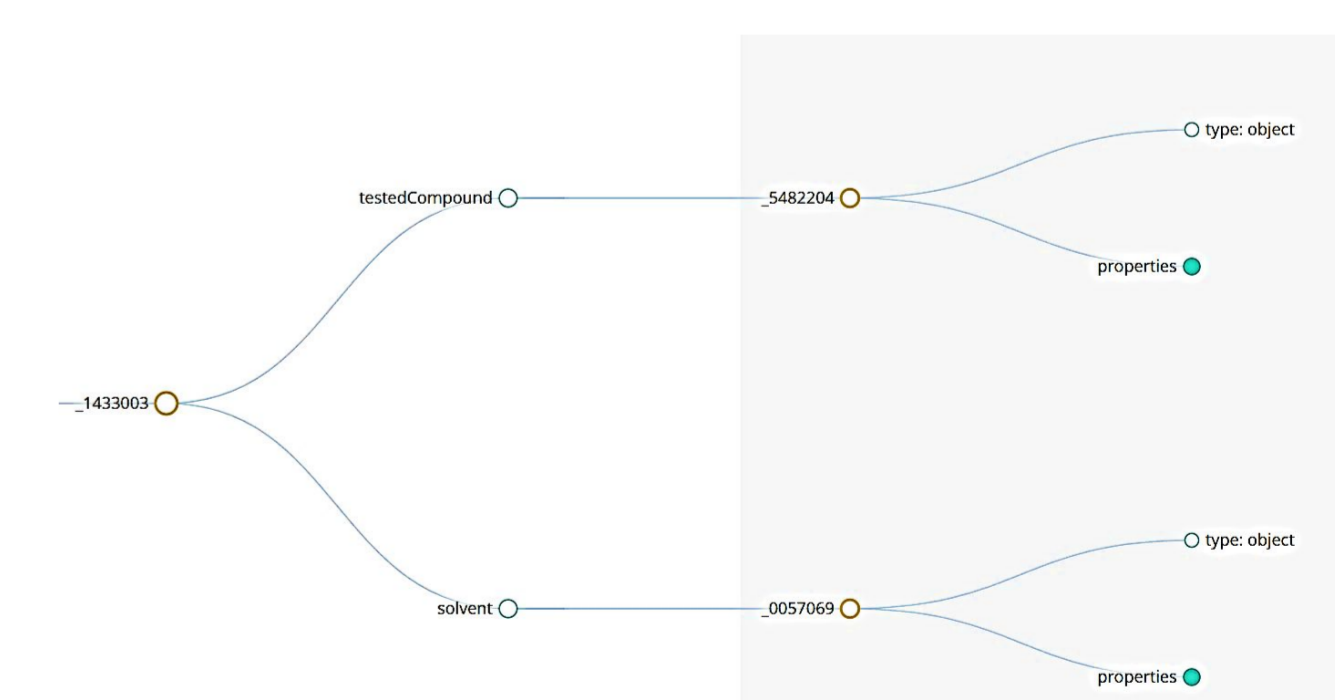## API design concept and semantic interoperability

OpenRiskNet will make the interfaces smarter by adding a **semantic interoperability layer**. By querying this layer, a service will provide
- scientific background of the service (link to the publication, manuals, tutorials and other training materials)
- technical background (links to source code, installation instructions, license information and deployment options)
- capabilities of the service (type and amount of generated output including the options and parameters)
- requirement on input data types and formats and options on the output format.

The semantic layer is realized as a combination of OpenAPI definitions with JSON-LD data serialization to bridge the worlds of API development and the semantic web.

References and more information

Elisabet Berggren, Andrew White, Gladys Ouedraogo, Alicia Paini, Andrea-Nicole Richarz, Frederic Y. Bois, Thomas Exner, Sofia Leite, Leo A. van Grunsven, Andrew Worth, Catherine Mahony, "Ab initio chemical safety assessment: A workflow based on exposure considerations and non-animal methods", Computational Toxicology, Volume 4, 2017, Pages 31-44.

https://openrisknet.org/development/api-concept/
https://openrisknet.org/development/case-studies/
https://json-ld.org/spec/latest/json-ld/
https://www.openshift.com/

Acknowledgements