OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE

Associated Partner Programme and Implementation Challenge

Lessons Learned

Thomas Exner (Edelweiss Connect GmbH)

OpenRiskNet: Open e-Infrastructure to Support Data Sharing, Knowledge Integration and *in silico* Analysis and Modelling in Risk Assessment
Project Number 731075

Goals of the Associated Partner Programme

- Strengthening the working ties between the OpenRiskNet Consortium members and other organisations within relevant scientific and technology communities.
- Open to any organisation such as a university, institute, consortium, non-governmental organisations (NGOs), as well as small and medium enterprises (SMEs) or large commercial companies
- 3 types of partners:
  a. service providers
  b. early adopters
  c. technology partners

Associated partners

List of associated partners

Service providers

Korea Institute of Toxicology

ToxPlanet

Hamburger Informatik Technologie-Center e.V. (HITeC)

NovaMechanics Ltd.

BIGCHEM GmbH

PROSILICO

Early adopters

University of Oxford

Diamond Light Source

Prof. Andrew Nelson, University of Leeds

Technology partners

Red Hat

Swedish National Infrastructure for Computing Science Cloud

Standard agreement

OpenRiskNet Associated Partner Programme Agreement

Version 1.4 for Service Providers

Between

(Name of Associated Partner)

and

Douglas Connect GmbH on behalf of the OpenRiskNet Consortium

hereinafter, jointly or individually, referred to as "Parties" or "Party"

Idea and issues with standard contract

- We wanted to be as open as possible with our associated partners allowing them to participate in consortium meetings and exchange confidential information → CDA needed
- OpenRiskNet is not legal entity and cannot sign contracts
- Consortium agrees that coordinator can sign on behalf of OpenRiskNet

- Especially for technology partners such a formal contract is not of big benefit → exchange of knowledge was still very active
- Small changes are requested by associated partners → standard contract not usable
- Other projects and other initiatives are also not legal entities

Goals of the Implementation Challenge

- Created to select external tools especially in areas of risk assessment not completely covered by the OpenRiskNet consortium
- Third parties can apply for partial financially and strongly technically support
- The scientific advisory board evaluates the proposed services and select the winning groups
- The winner is asked to become an associated partner

Challenge Session	Organisation	Contact Person	Email	Contact in OpenRiskNet	Contract with
31 October 2018	National Center for Computational Toxicology, US Environmental Protection Agency	Holly Mortensen	mortensen.holly@epa.gov	UM	EwC
	Korea Institute of Toxicology	Hyun Kil Shin	hyunkil.shin@kitox.re.kr	EwC	EwC
	ToxPlanet	Matthias Timberlake	mtimberlake@toxplanet.com	UM/EwC	EwC
	BIGCHEM GmbH	Igor Tetko	itetko@bigchem.de	JGU	EwC
15 July 2019	Hamburger Informatik Technologie-Center e.V. (HITeC)	Johannes Kirchmair	johannes.kirchmair@uib.no	VU	EwC
31 January 2019	Prosilico	Urban Fagerholm	urban.fagerholm@prosilico.com	UU	EwC
	NovaMechanics Ltd	Antreas Afantitis	afantitis@novamechanics.com	NTUA	EwC
	Diamond Light Source Ltd. / Informatics Matters Ltd.	Rachael Skyner	rachael.skyner@diamond.ac.uk	IM	EwC
		Frank von Delft	frank.von-delft@diamond.ac.uk		
30 April 2019	Princess Margaret Bioinformatics and Computational Genomics Laboratory, University Health Network, Toronto, Canada	Benjamin Haibe-Kains	bhaibeka@uhnresearch.ca	UM	EwC
	Leiden University	Katy Wolstencroft	k.j.wolstencroft@liacs.leidenuniv.nl	UM	EwC

Partner services

OCHEM models

IN PROGRESS

Prediction of chemicals

Prediction of different endpoints

Provided by: BigChem GmbH
Type: Trained model
Applicability domain: Predictive toxicology
Topic: Chemical properties, Risk assessment, Structure-activity relationship (SAR / QSAR), Predictive modelling
Biological area: NOAEL/LOAEL, Acute toxicity

✓ For end-users

DETAILS → VISIT SERVICE →

ToxicoDB

IN PROGRESS

A database for curated toxicogenomic datasets

ToxicoDB isa web-application based on the code base of the existing PharmacoDB web-application. The ToxicoDB web-app will provide an intuitive interface for all users (including users that are not computational ...

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

✓ For end-users
✓ For developers

DETAILS → VISIT SERVICE →

nanoQSAR model for the prediction of the cellular uptake and the virtual screening of nanoparticles via Enalos Platform

INTEGRATED

Enalos Platform nanoinformatics nanoparticles

A validated predictive model for nanoparticles cellular uptake, that is part of the Enalos infrastructure deployed into the OpenRiskNet reference environment. The model can be used for the predictions of ...

Provided by: NovaMechanics Ltd
Type: Trained model, Model
Applicability domain: Computational modelling, Toxicology, Predictive toxicology
Topic: Nano safety, Risk assessment, Structure-activity relationship (SAR / QSAR), Predictive modelling

✓ For end-users
✓ For developers

DETAILS → VISIT SERVICE →

Prosilico's Human In Vivo ADME/PK-Prediction Studio

IN PROGRESS

Predict ADME/PK with Confidence

The service predicts 8 basic human clinical ADME/PK-parameters directly from molecular structure and can also be used to optimize ADME/PK-characteristics of drug candidates.

Provided by: Prosilico
Type: Application, Software, Service
Applicability domain: Predictive toxicology
Topic: Kinetics, Structure-activity relationship (SAR / QSAR), Predictive modelling
Biological area: Toxicokinetics

✓ For end-users

Nanoinformatics Tool for the Virtual Screening of Metal Oxide Nanoparticles via Enalos Platform

INTEGRATED

Virtual Screening Metal Oxide Nanoparticles Enalos Platform

A predictive classification model for the toxicological assessment of iron oxide NPs with different core, coating and surface modification based on a number of different properties including size, relaxivities, zeta ...

Provided by: NovaMechanics Ltd
Type: Application, Trained model, Model, Service
Applicability domain: Computational modelling, Toxicology, Predictive toxicology
Topic: Nano safety, Risk assessment, Structure-activity relationship (SAR / QSAR), Predictive modelling

✓ For end-users
✓ For developers

FAME 2 site-of-metabolism predictor

IN PROGRESS

Machine learning models for site-of-metabolism prediction

FAME 2 is a cytochrome P450 site-of-metabolism predictor that uses extra trees machine learning models based on circular 2D atomic descriptors. FAME (FAst MEtabolizer) is currently being used at several ...

Provided by: Universitaet Hamburg and UCT Prague and University of Bergen
Type: Application, Software, Trained model, Model, Service
Applicability domain: Predictive toxicology
Topic: Structure-activity relationship (SAR / QSAR), Predictive modelling

✓ For end-users

How to fund the Implementation Challenge

- Specific budget was allocated for winners
- No mechanism in H2020 to add partners and tasks during the project
  - ➢ not subcontracting but in kind work
  - ➢ generic task - but this was similar to the service integration task anyway
- After Programme and Financial Officer as well as auditor feedback, secondment contract was identified as best method

Implementation Challenge contract

EdelweissConnect

Secondment Agreement

between

University Health Network
101 College Street, Suite 150, Heritage Building, MaRS Centre, Toronto, ON, M5G 1L7, Canada

(the "**seconding organisation**"" or "**UHN**")

and

Edelweiss Connect GmbH,
Hochbergerstrasse 60C, 4057 Basel, Switzerland

(the "**hosting organisation**")

hereinafter jointly also the "**Parties**" and each a "**Party**"

Whereas, the seconding organisation will second the Secondees (as defined below) in accordance with and subject to the terms of this Agreement.

Whereas, the seconding organisation is an Ontario not-for-profit corporation incorporated under the *University Health Network Act*, 1997, S.O. 1997, c. 45,

Whereas, the hosting organisation is a limited liability company organised and existing vitzerland, registered in the commercial register of the Canton of

“Issues” with Implementation Challenge

- Complex drafting of the contract
- Little experience of consortium partners’ administrations to handle such contracts
- Contract with organization but not individuals
- IP discussions (only descriptions and interfaces as part of the contracts)

- Even if it took a while, associated partners worldwide could agree on the contracts with only minor changes
- Clear rules for monitoring, reporting and payment even if this puts additional burden on the coordinator

Alternatives?

- Transnational access (infrastructure projects, services offered to associated partners)
- Funding of specific activities of working groups (funding for technical developments?)
- ...