International Cooperation in Sustainable Open Science Knowledge Infrastructure Supporting Predictive Toxicology and Risk Assessment

Barry Hardy (Edelweiss Connect)

3rd In Silico Toxicology Conference 2022

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Barry.Hardy@edelweissconnect.com

Image source: https://postdoc.uni-graz.at/de/veranstaltungen/detail/article/why-do-open-science/

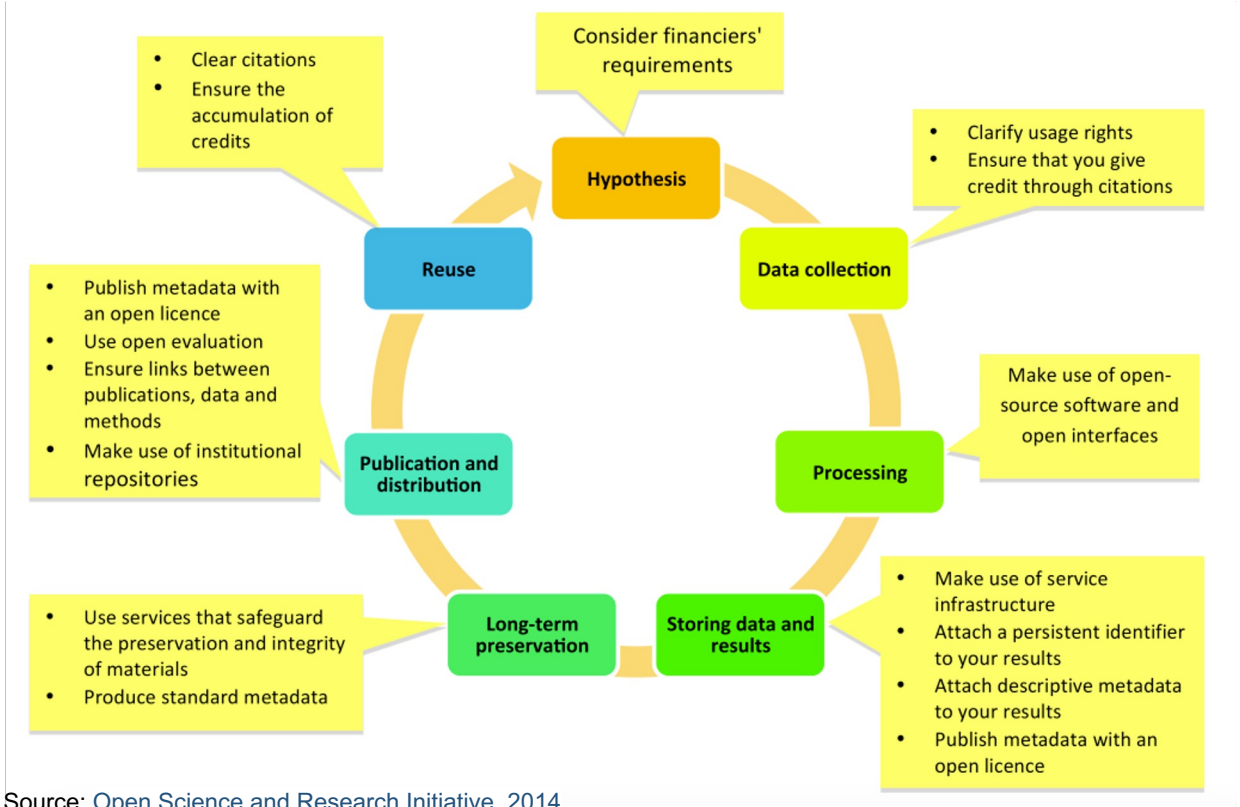
What is OpenScience?

Open science encompasses unhindered access to scientific articles, access to data from public research, and collaborative research enabled by ICT tools and incentives.

Broadening access to scientific publications and data is at the heart of open science, so that research outputs are in the hands of as many as possible, and potential benefits are spread as widely as possible.

https://www.oecd.org/sti/inno/open-science.htm

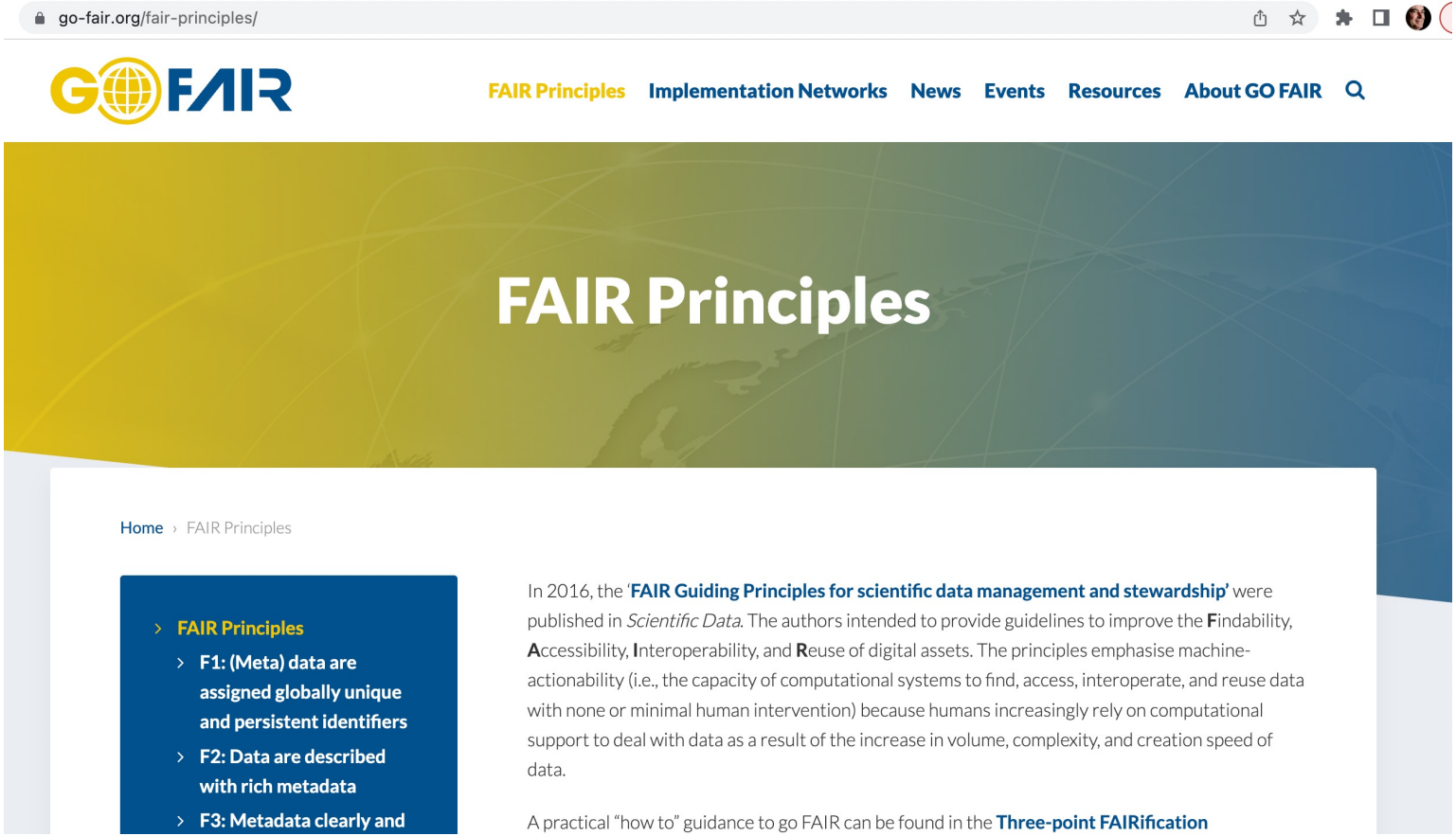
Promoting openness at different stages of the research process



Source: Open Science and Research Initiative, 2014

Open Science is about **extending the principles of openness to the whole research cycle**, fostering sharing and collaboration as early as possible thus entailing a systemic change to the way science and research is done.

FAIR Principles



OpenScience Taxonomy

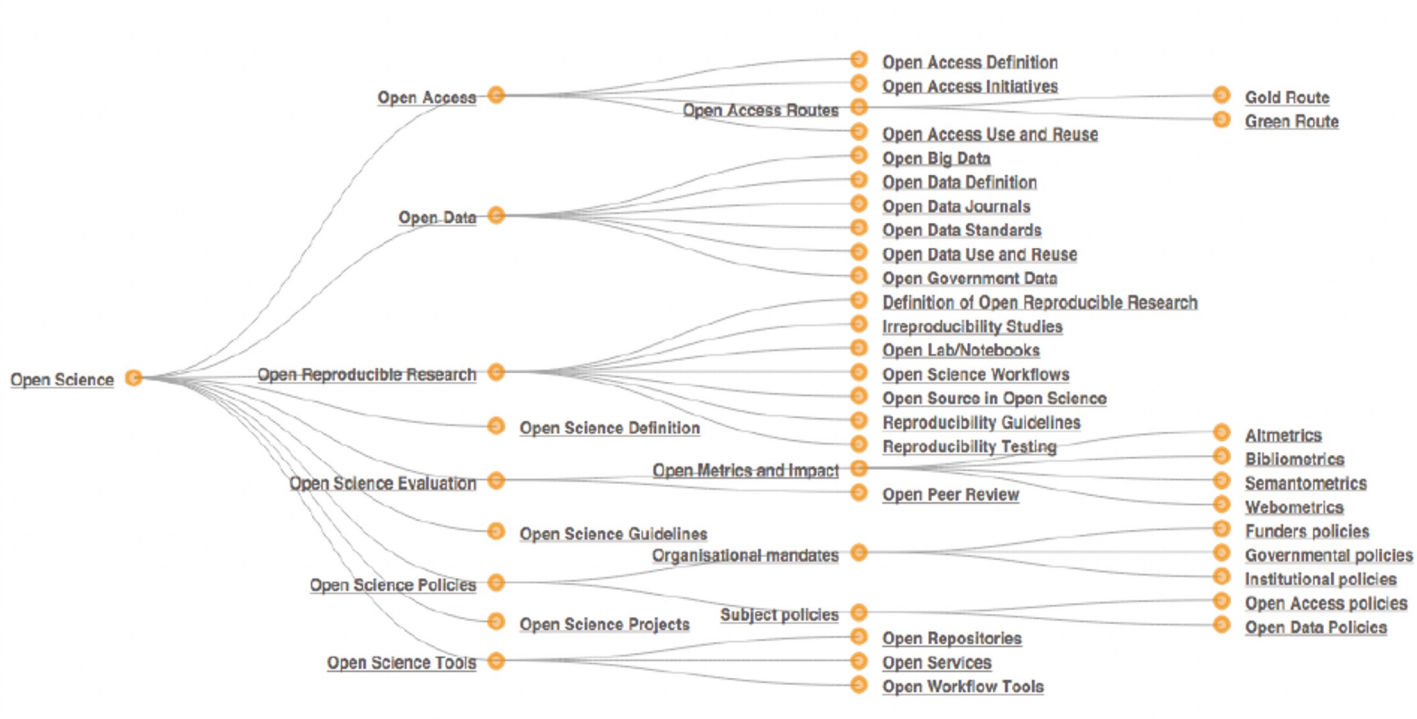
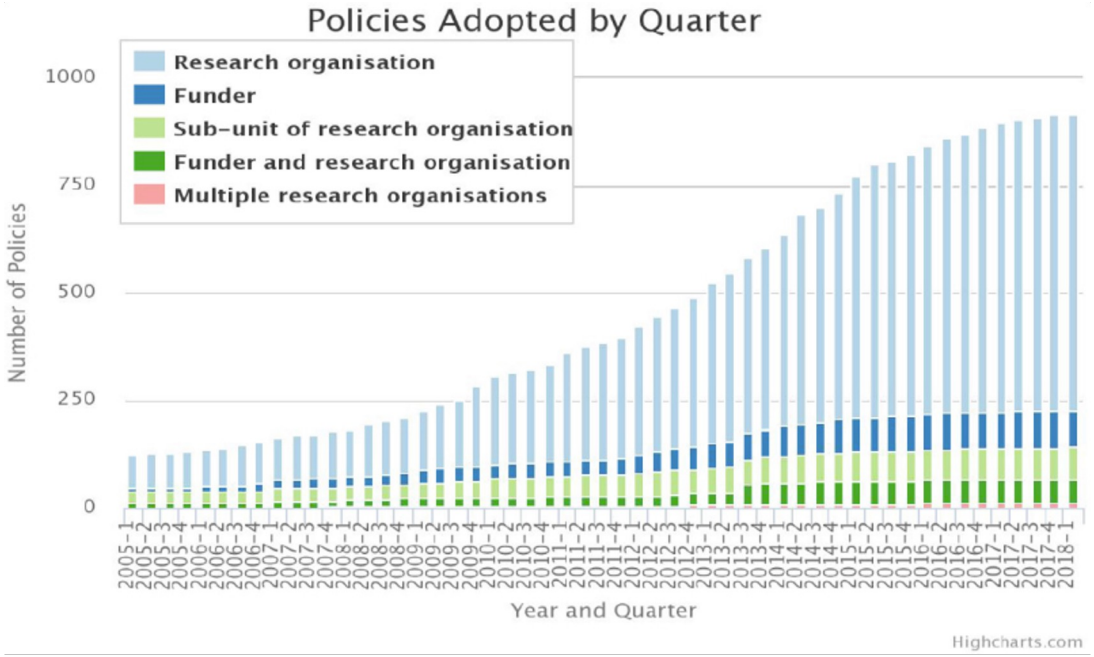


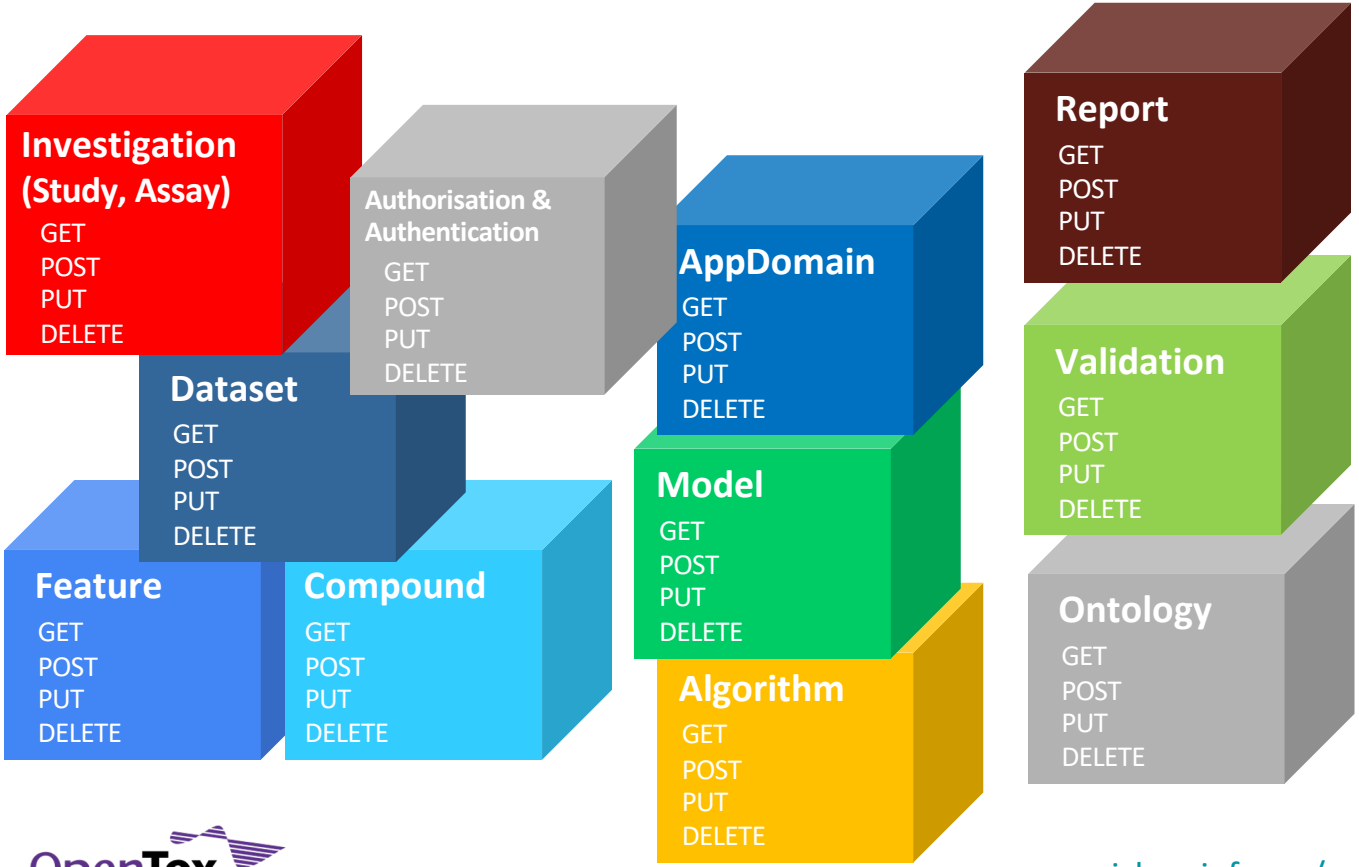
Image source: [Pontika et al., 2015]

Open science policies adopted by research funders and research organizations around the world



Source: ROARMap, University of Southampton (embedded as a figure in the following book: https://www.ncbi.nlm.nih.gov/books/NBK525413/

OpenTox and Open Components and Standards (Proposed 2010)



OpenTox

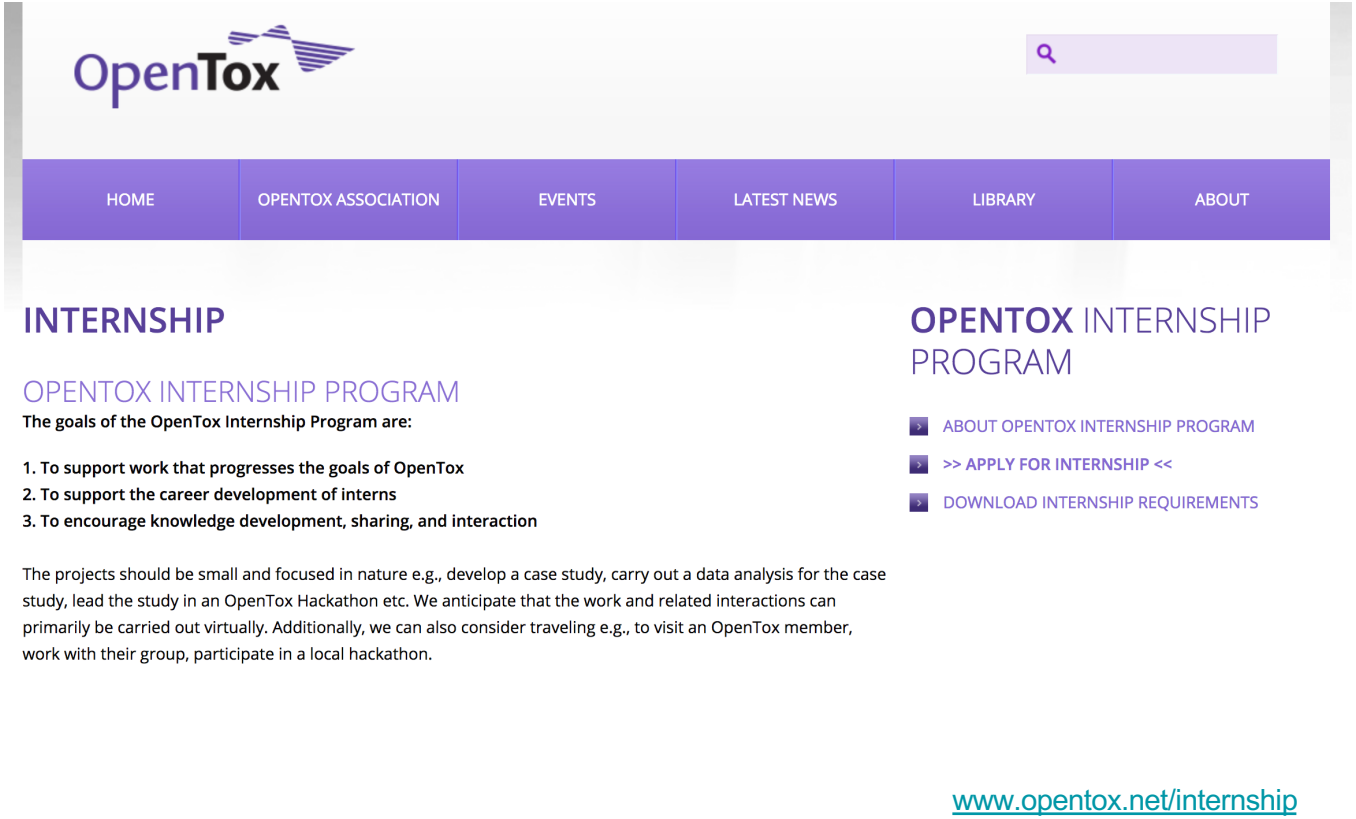
www.jcheminf.com/content/2/1/7

Consensus on need for Common Language and Ontology

- See perspectives and roadmap published in A Toxicology Ontology Roadmap ALTEX 29(2), 129- 137 and Toxicology Ontology Perspectives 139 - 156 (2012)
- Available online in Open Access mode from www.altex.ch
- Barry Hardy (Douglas Connect and OpenTox), Gordana Apic (Cambridge Cell Networks), Philip Carthew (Unilever), Dominic Clark (EMBL-EBI), David Cook (AstraZeneca), Ian Dix (AstraZeneca & Pistoia Alliance), Sylvia Escher (Fraunhofer Institute for Toxicology & Experimental Medicine), Janna Hastings (EMBL-EBI), David J. Heard (Novartis), Nina Jeliazkova (Ideaconsult), Philip Judson (Lhasa Ltd.), Sherri Matis-Mitchell (AstraZeneca), Dragana Mitic (Cambridge Cell Networks), Glenn Myatt (Leadscope), Imran Shah (US EPA), Ola Spjuth (University of Uppsala), Olga Tcheremenskaia (Istituto Superiore di Sanità), Luca Toldo (Merck KGaA), David Watson (Lhasa Ltd.), Andrew White (Unilever), Chihae Yang (Altamira)

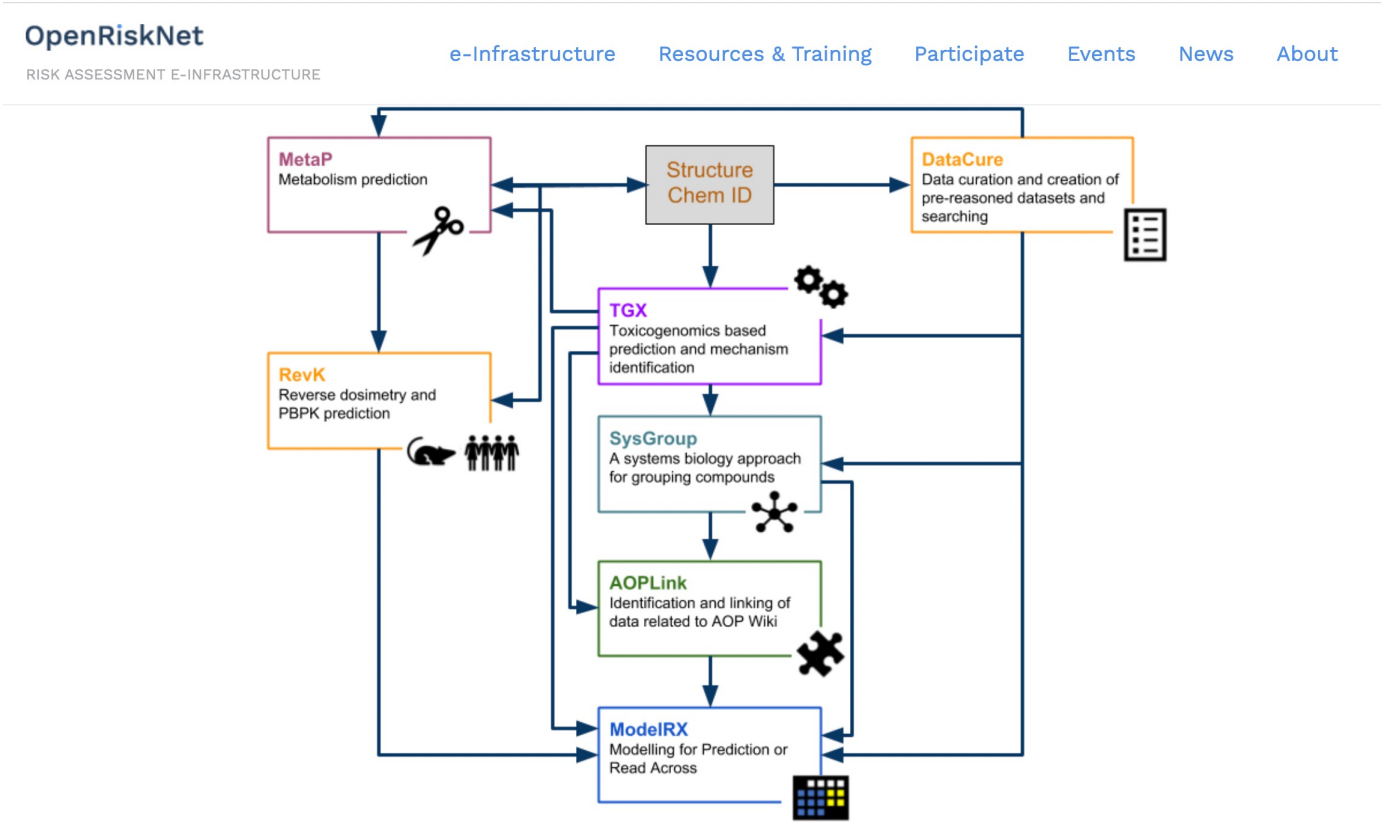
*Based on Proceedings from the **Toxicology Ontology Roadmap Workshop***
EMBL-EBI Industry Programme Workshop
16 -17th November 2010, Hinxton, UK

OpenTox Association



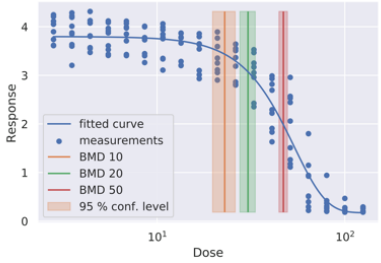
www.opentox.net/internship

OpenRiskNet – Integrated services and use cases



https://openrisknet.org/

Knowledge Management on EU-ToxRisk



Harmonised Data, Protocol and Metadata Management Infrastructure supported by EdelweissData

Data and Knowledge Management on EUToxRisk program

Experiments
Generates 'raw data'
- *e.g.* Fluorescent intensities

Data processing
Process raw data
- Fluorescent intensities → activities
- Experiment/laboratory specific

Data summarization
Summarize processed data
- Activities → curve fit → *p*XC50
- Common approaches?

Test Method DB
Stores detailed description of test methods including SOPs
- *Human readable description*
- *Computer-readable annotations*

BioStudies @ EMBL-EBI
Data repository and archive
- Data stored as individual data sets

Knowledge Sharing
Test method and data portal
- Data reformatted to optimize querying
- *e.g.* join data across compounds

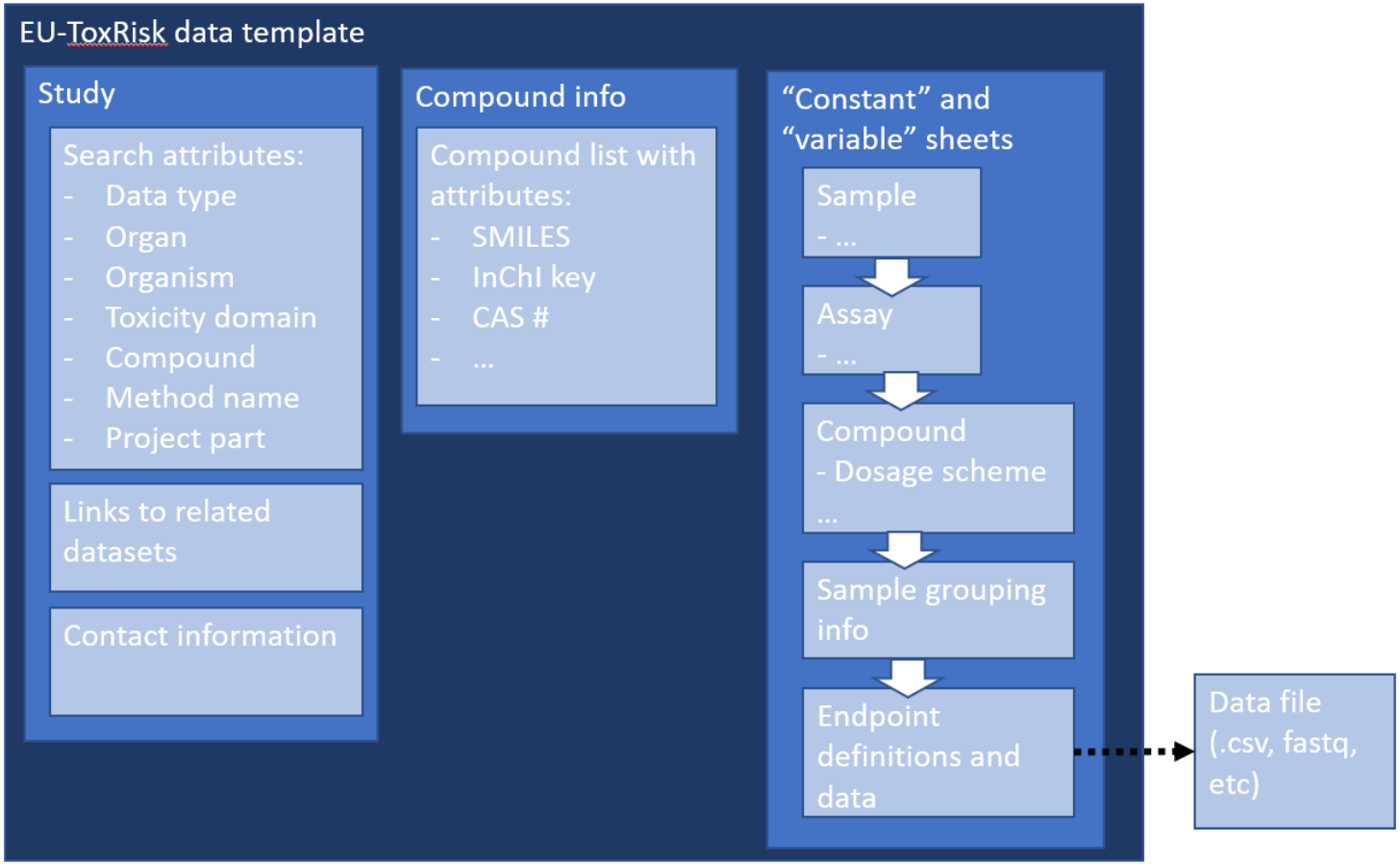
Modelling
Statistical model building
- Requires summarized data

Visualization
Exploratory data analysis
- Summarized data linked to underlying data

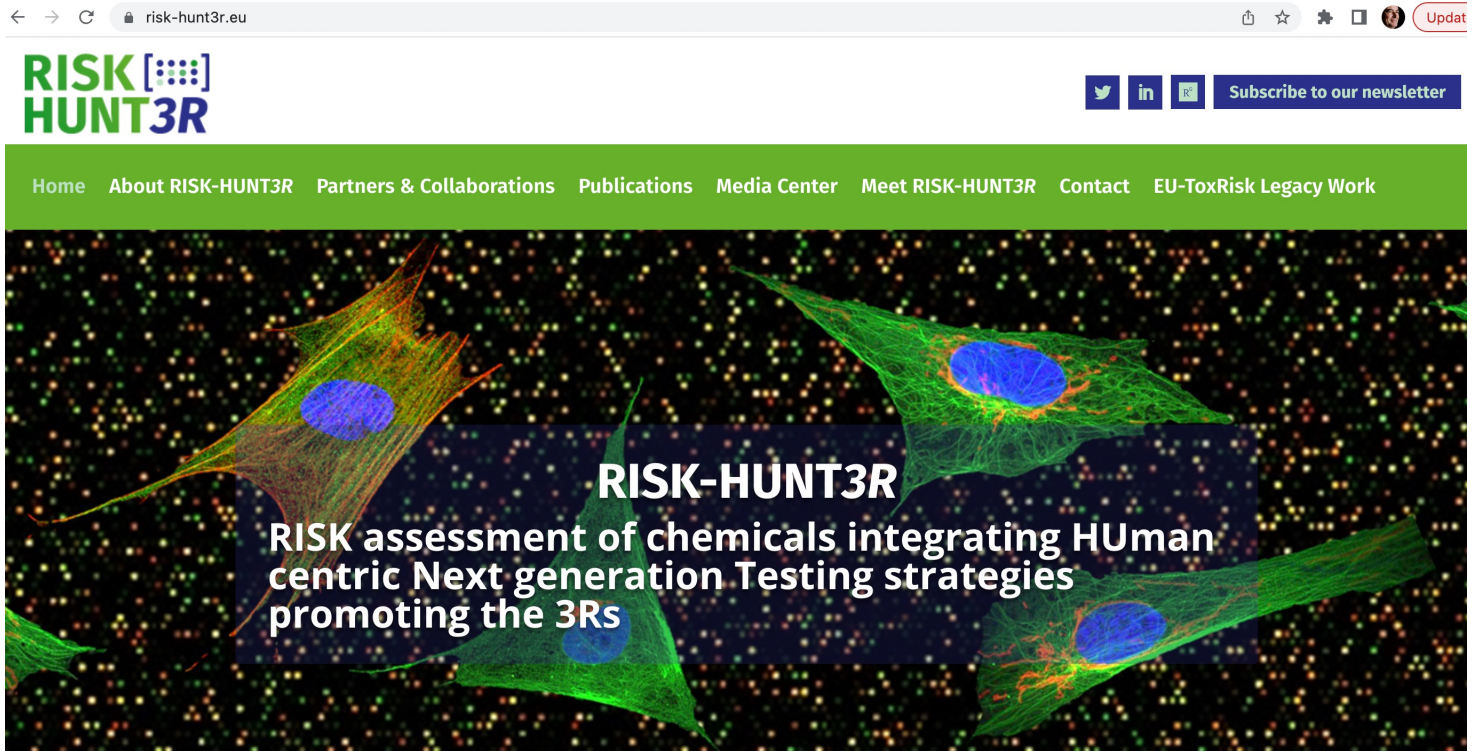
Decision making
Weight of evidence
- Model output
- Expert opinion
- ...

Raw data
Processed data
Summary data
Metadata

Data Generation template

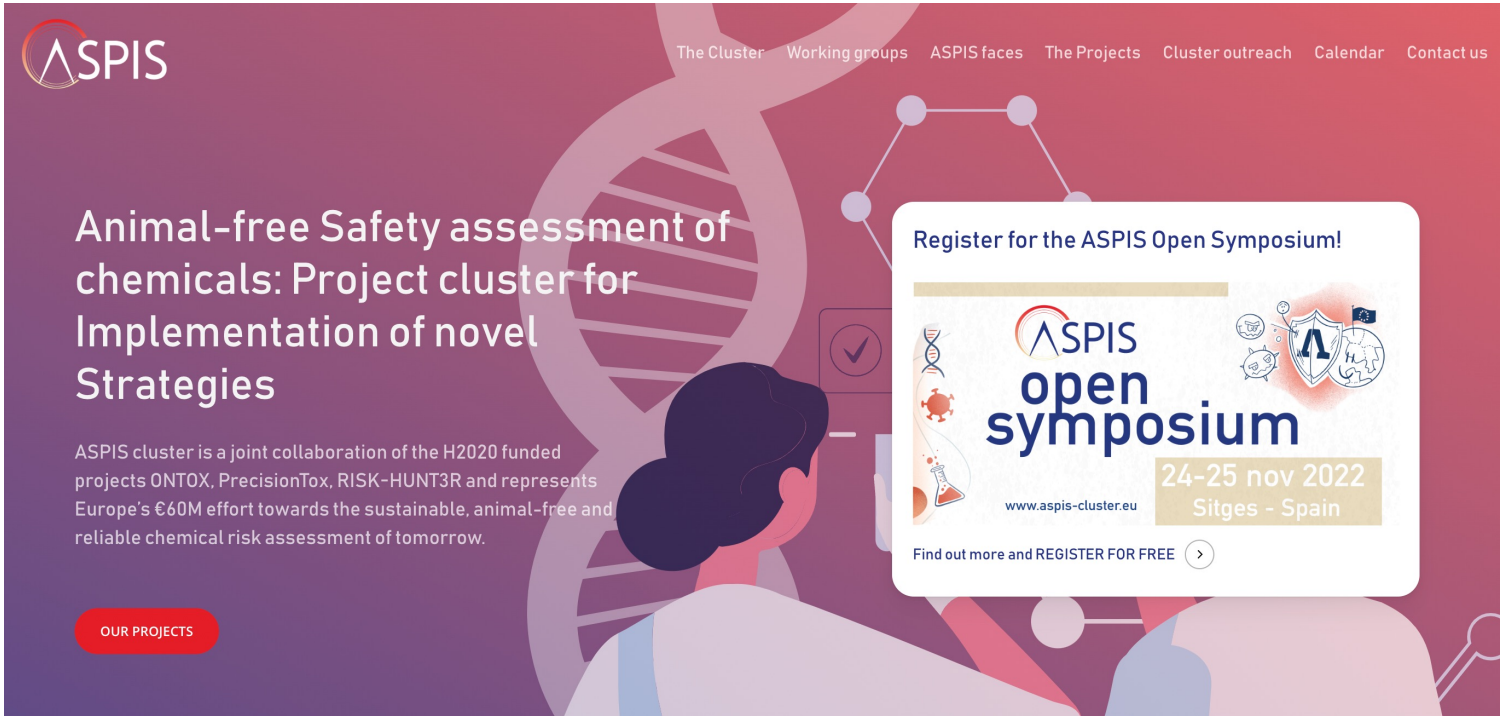


RISK-HUNT3R (2021 – 2026)



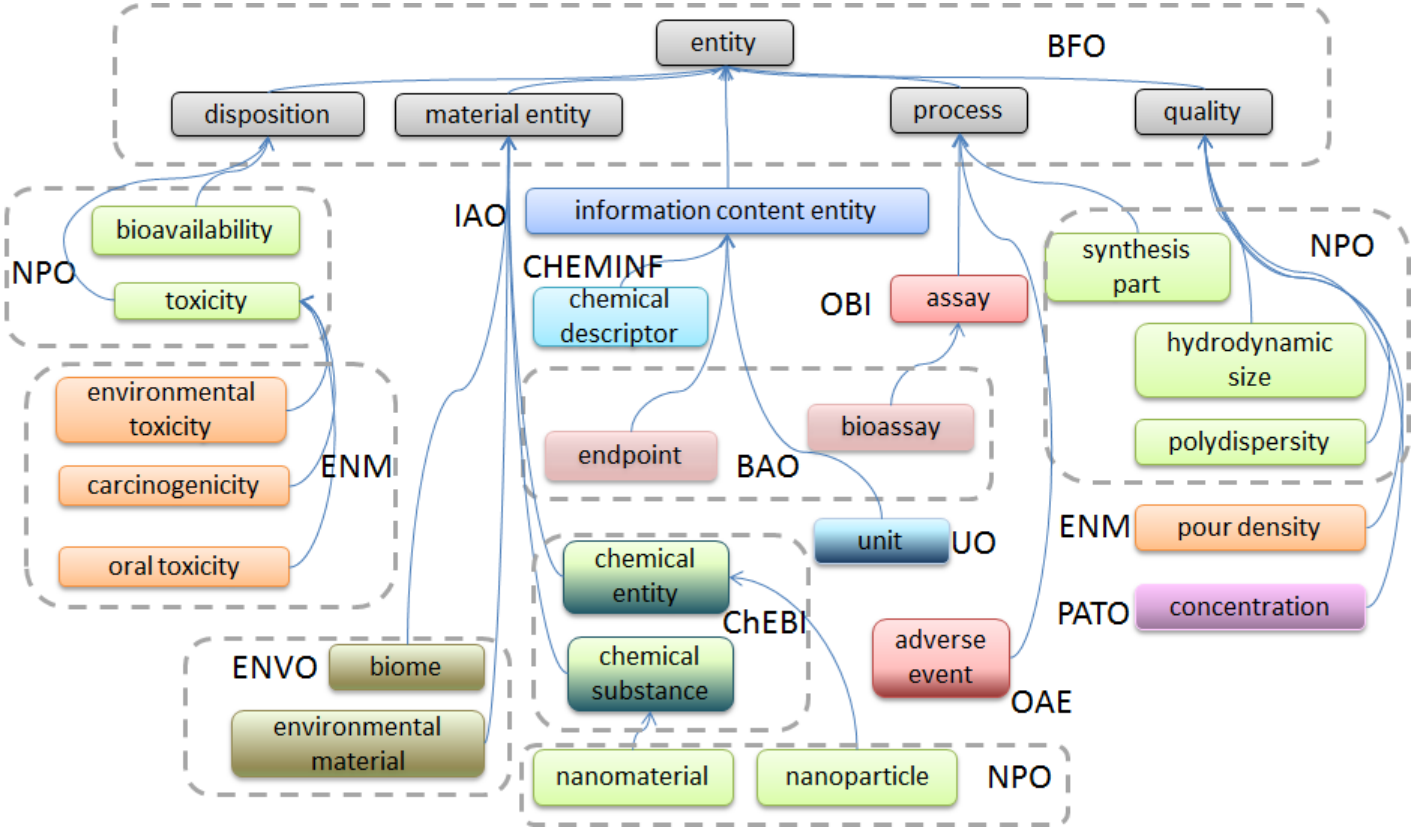
https://www.risk-hunt3r.eu/

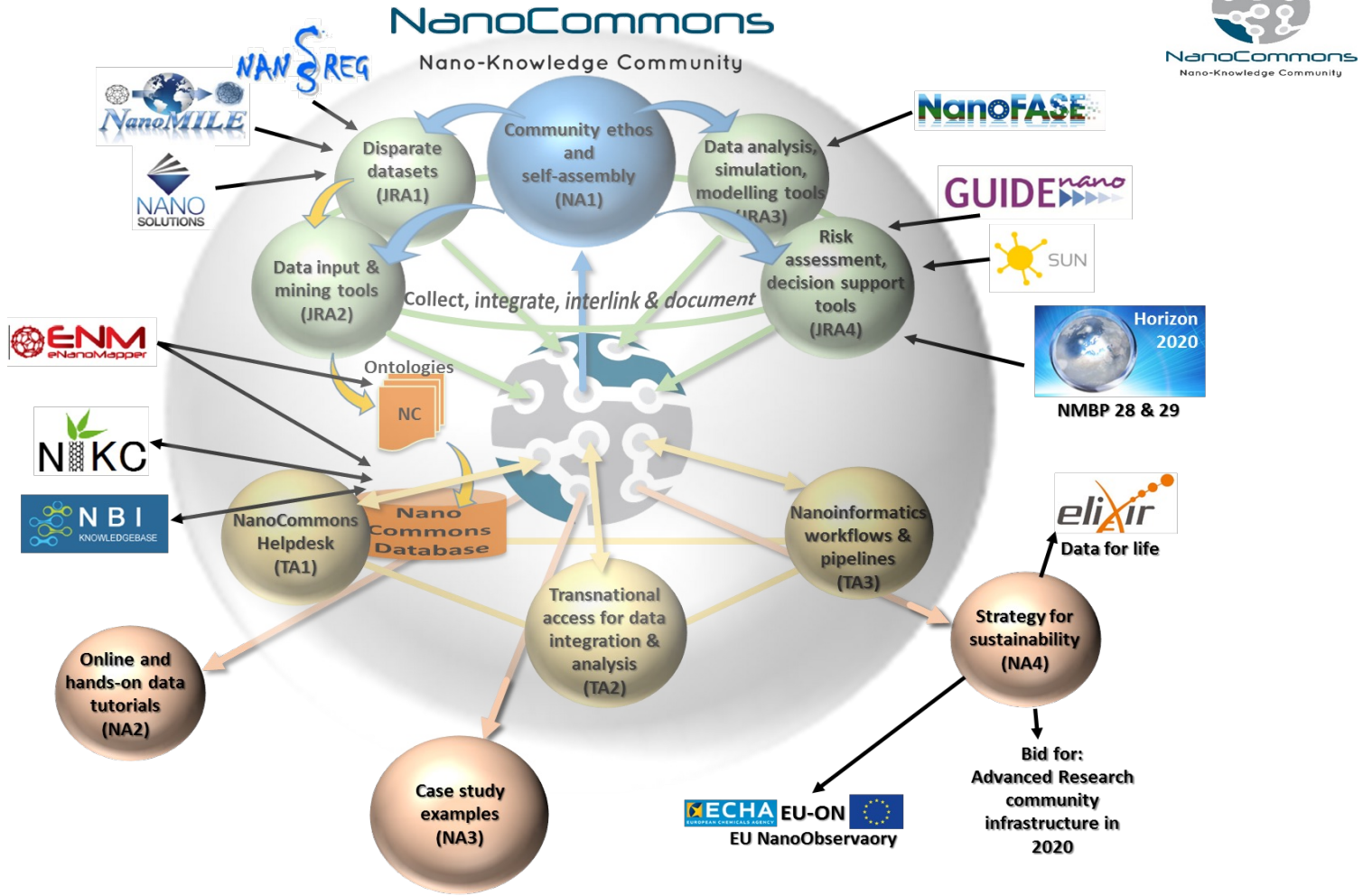
ASPIS Cluster (ONTOX, Precision Tox, RISK-HUNT3R) (2021-2026)



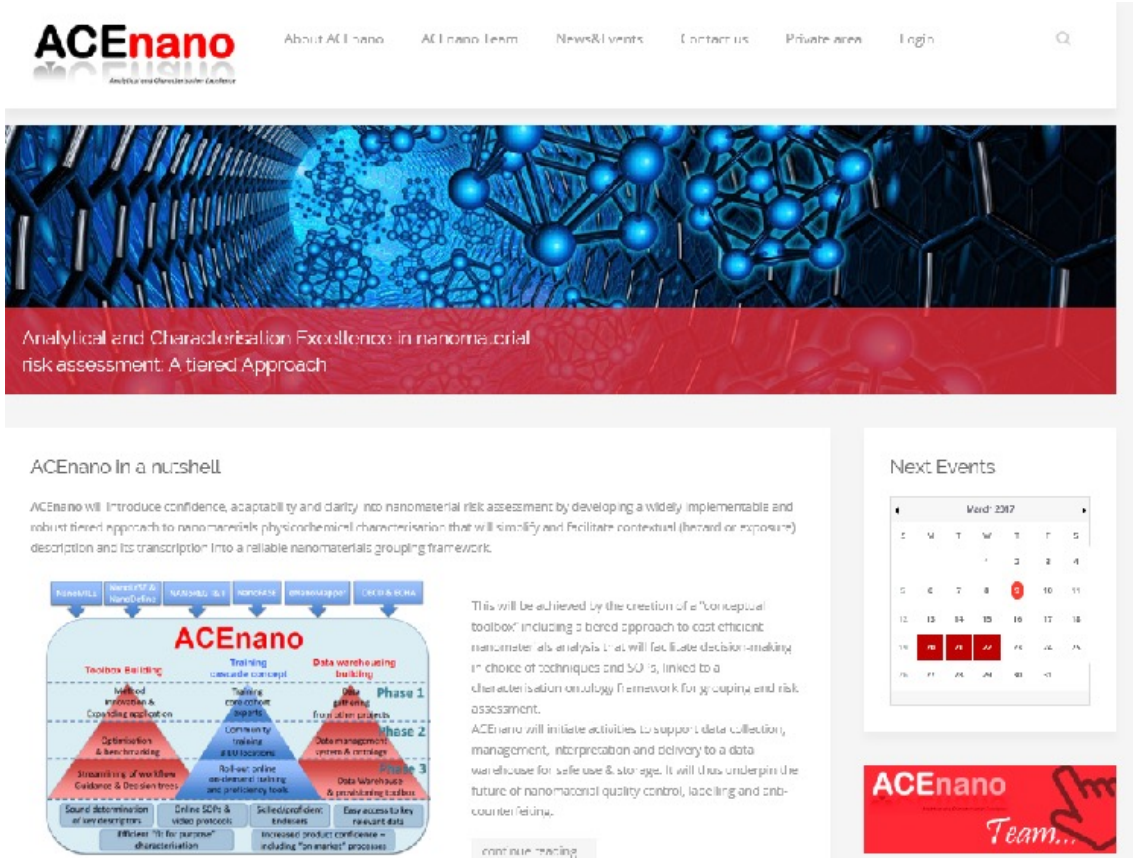
https://aspis-cluster.eu/

ENanoMapper Ontology



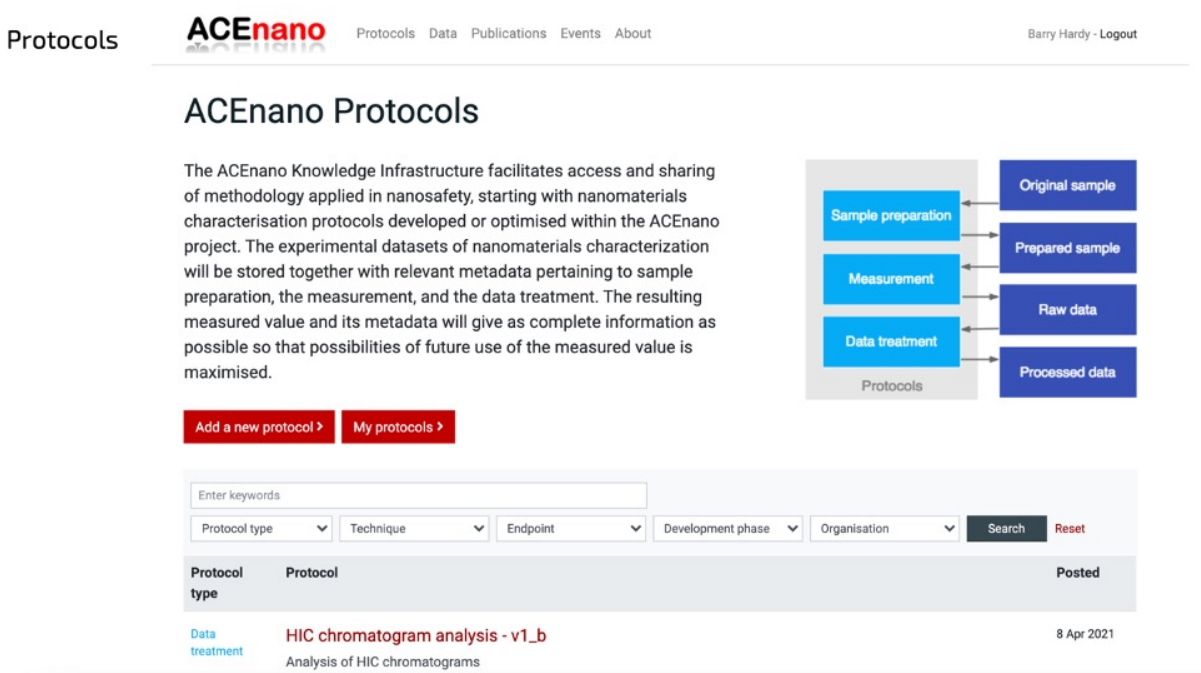

NanoCommons
Nano-Knowledge Community
NANOREG
NanoMILE
NANO SOLUTIONS
NanoFASE
GUIDEnano
SUN
Horizon 2020
NMBP 28 & 29
eNM eNanoMapper
NIKC
NBI KNOWLEDGEBASE
elixir
Data for life
Disparate datasets (JRA1)
Community ethos and self-assembly (NA1)
Data analysis, simulation, modelling tools (JRA3)
Data input & mining tools (JRA2)
Collect, integrate, interlink & document
Risk assessment, decision support tools (JRA4)
Ontologies
NC
NanoCommons Helpdesk (TA1)
Nano Commons Database
Nanoinformatics workflows & pipelines (TA3)
Transnational access for data integration & analysis (TA2)
Strategy for sustainability (NA4)
Online and hands-on data tutorials (NA2)
Case study examples (NA3)
ECHA EU-ON
EU NanoObservaory
Bid for: Advanced Research community infrastructure in 2020

AceNano Characterisation Infrastructure

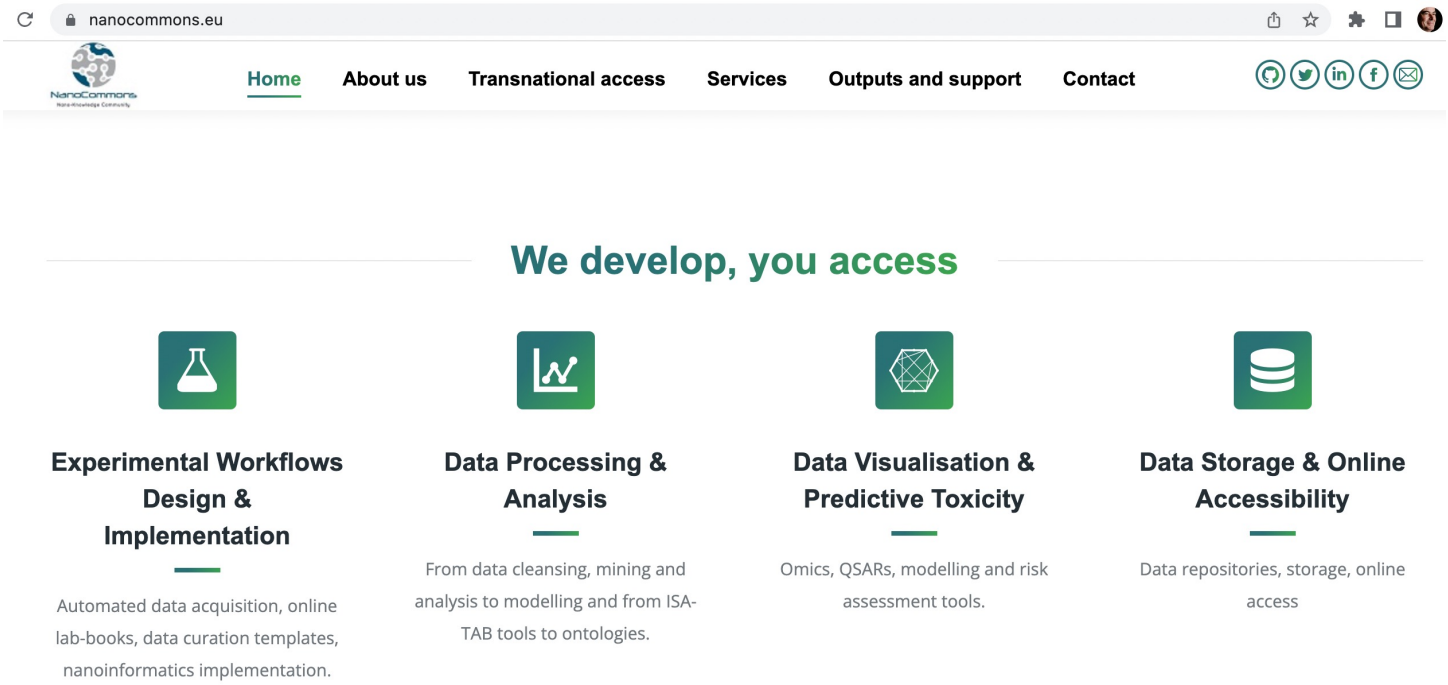


www.acenano-project.eu

Protocol Management

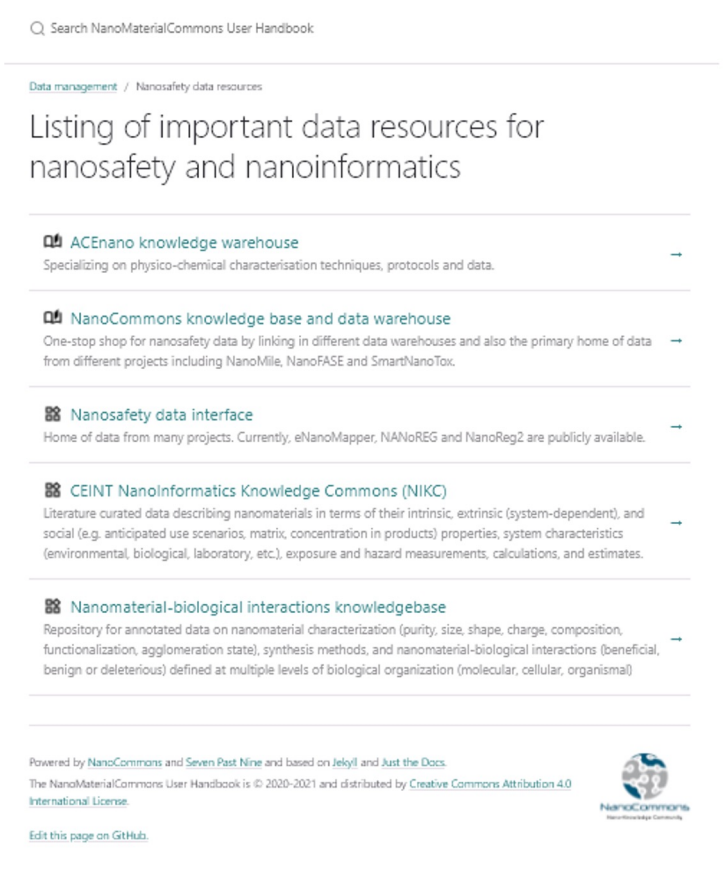


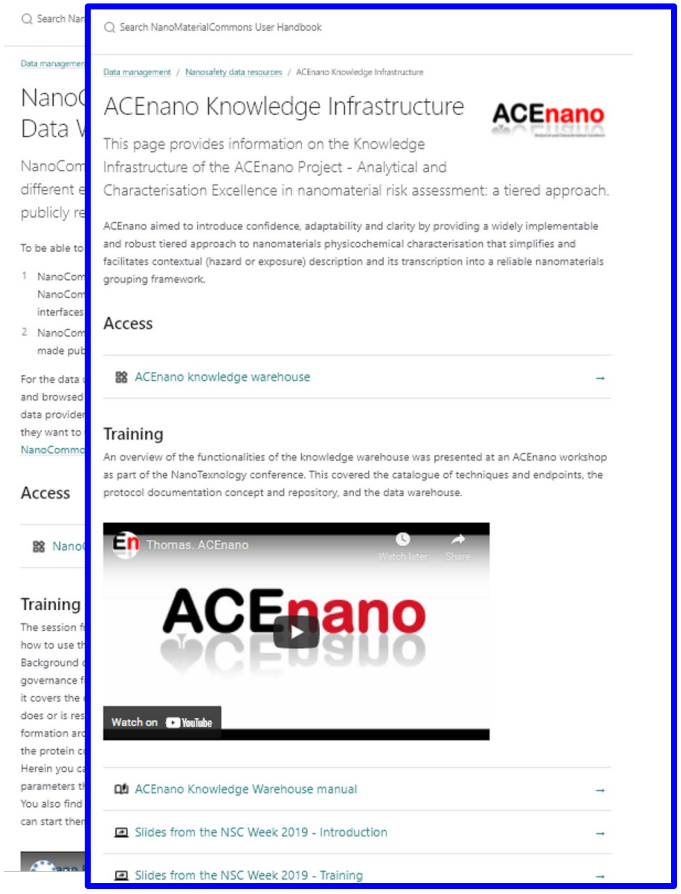
NanoCommons Knowledge Hub



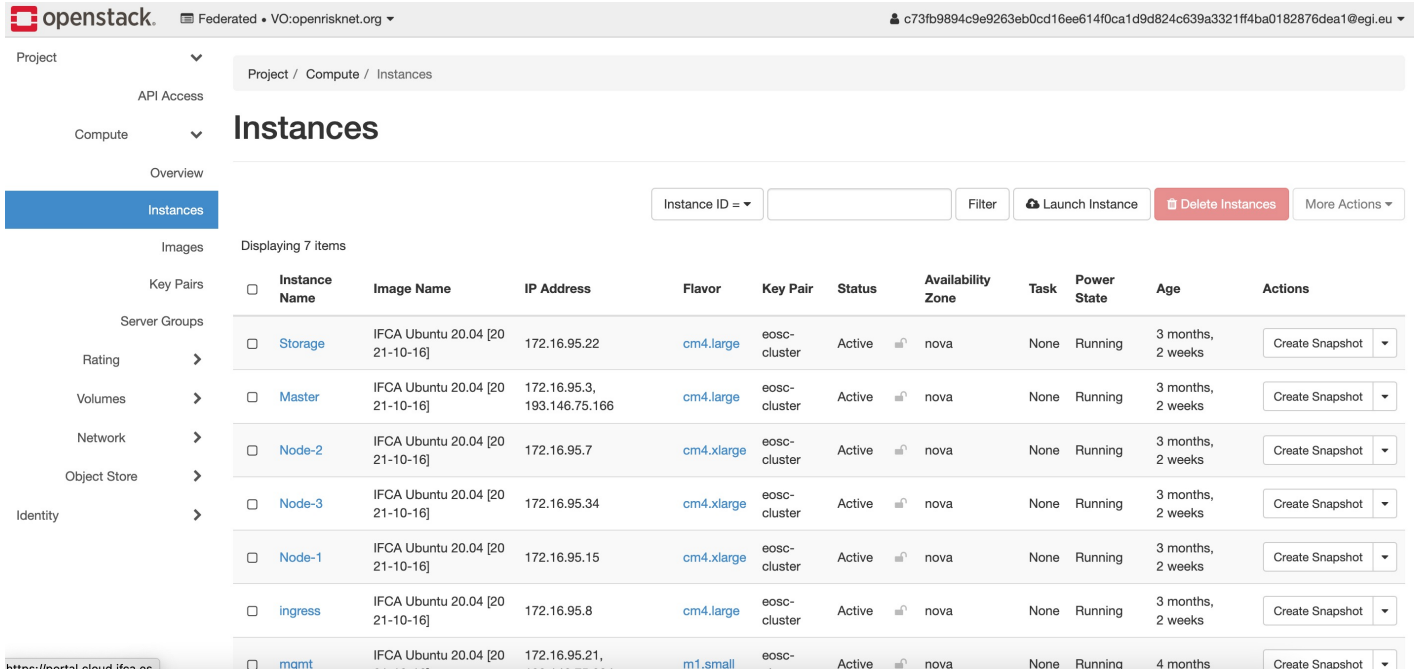
https://www.nanocommons.eu/

NanoCommons User guidance handbook



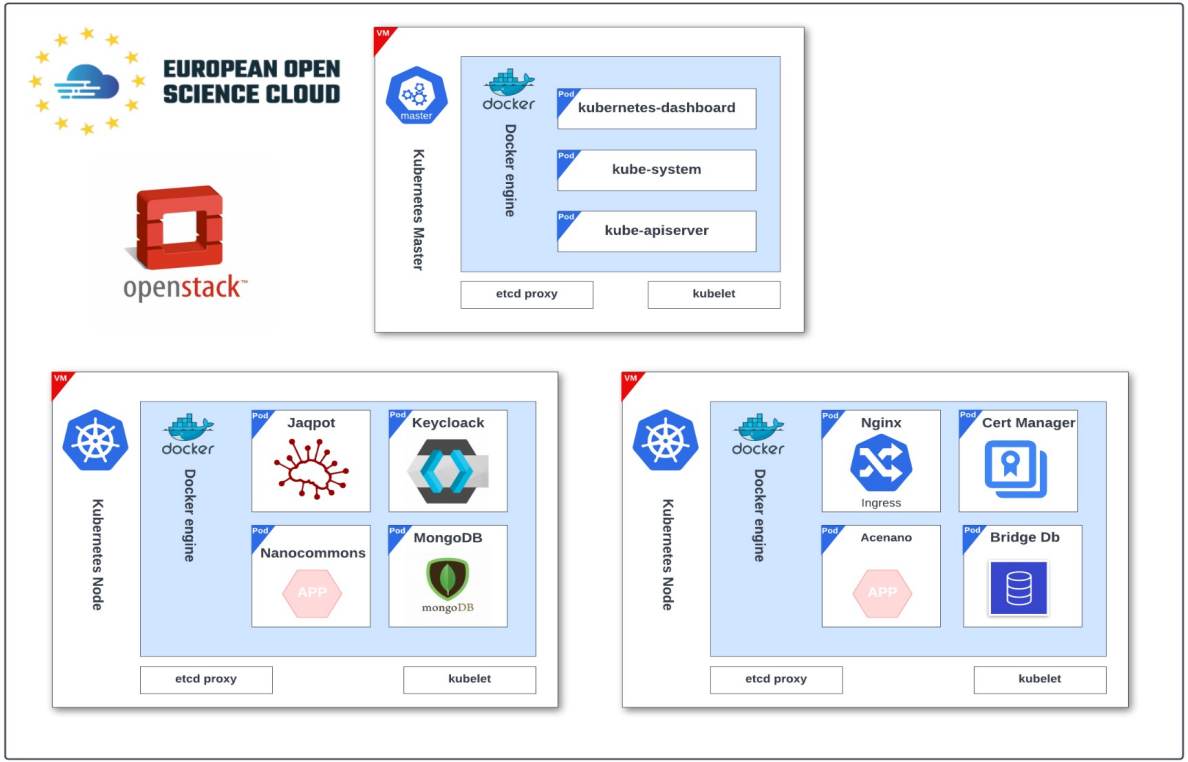


EOSC Cluster Configuration for Open Reources from OpenRiskNet/OpenTox/NanoCommons/EU-ToxRisk …. (2022)

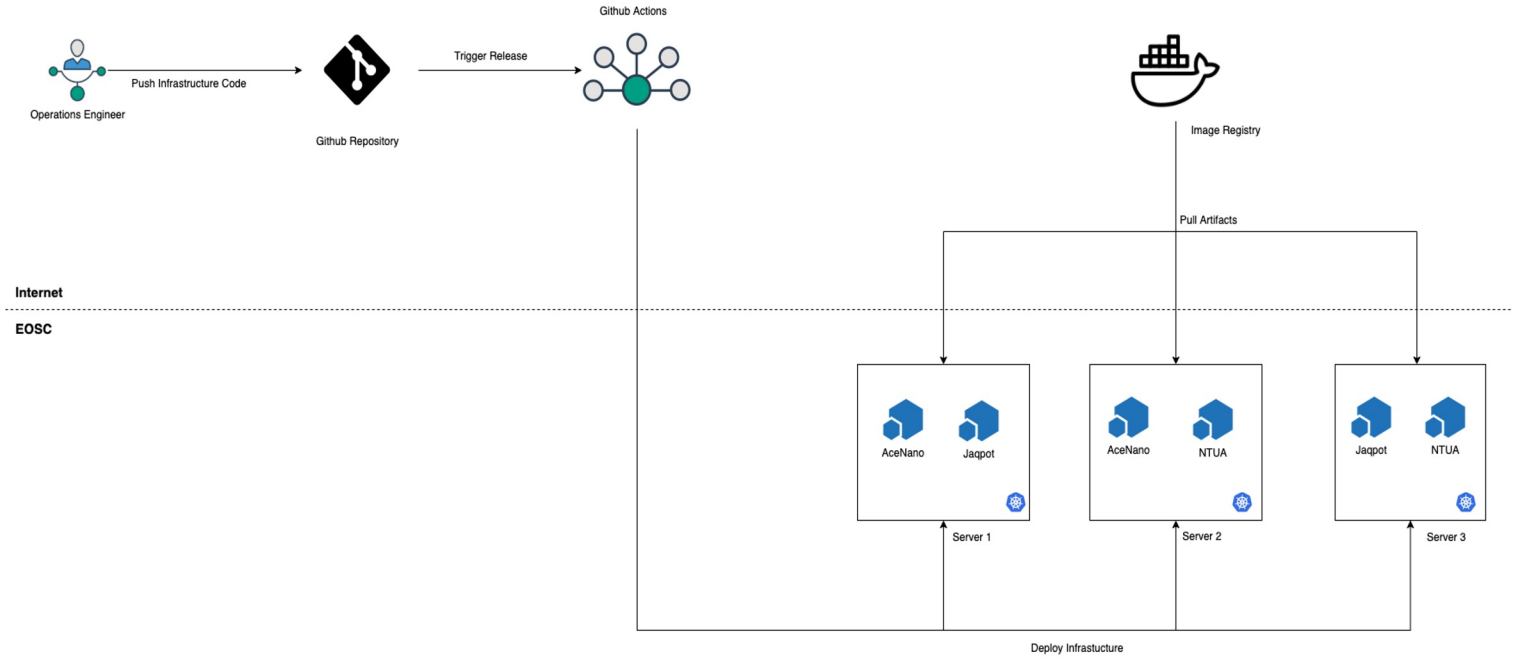


Goal is to establish a sustainable collaborative open knowledge infrastructure in predictive toxicology and risk assessment

EOSC Architecture for Orchestration and Deployment



EOSC Deployment Flow



Participation in Collaborative Knowledge Infrastructure Development

Open Toxicology and Risk Assessment Knowledge Infrastructure

We have started a collaborative initiative to create an open science knowledge infrastructure supporting community goals in predictive toxicology, risk and safety assessment. The goal is to work together to provide an increasing critical mass of working resources (databases, software, services, methods, tools, applications) including goals of usability, deployment, support, performance, security, interoperability and access to FAIR data to support users in their work. We plan to build as much as possible on existing initiatives such as OpenTox, OpenRiskNet, NanoCommons etc. to establish a stronger combined set of resources such as can be supported on the emerging European Open Science Cloud infrastructure. We will also consider collaboration with similar initiatives and goals in other regions. This questionnaire aims to obtain your feedback on interest in participation in such a venture as a resource developer and/or user.

barry@edelweissconnect.com Switch account

* Required

Form to express interest to be involved in our Open Knowledge Infrastructure initiative in predictive toxicology and risk assessment

https://forms.gle/bNCqZqu8Ln2pFnMk9

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3rd In Silico Toxicology Conference 2022
29 September 2022
Barry.Hardy@edelweissconnect.com

https://www.linkedin.com/in/barryhardy/

Interest in Knowledge Infrastructure Participation Form:
https://forms.gle/bNCqZqu8Ln2pFnMk9