



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

Barry Hardy (Edelweiss Connect)  
3rd In Silico Toxicology Conference 2022  
29 September 2022  
Barry.Hardy@edelweissconnect.com

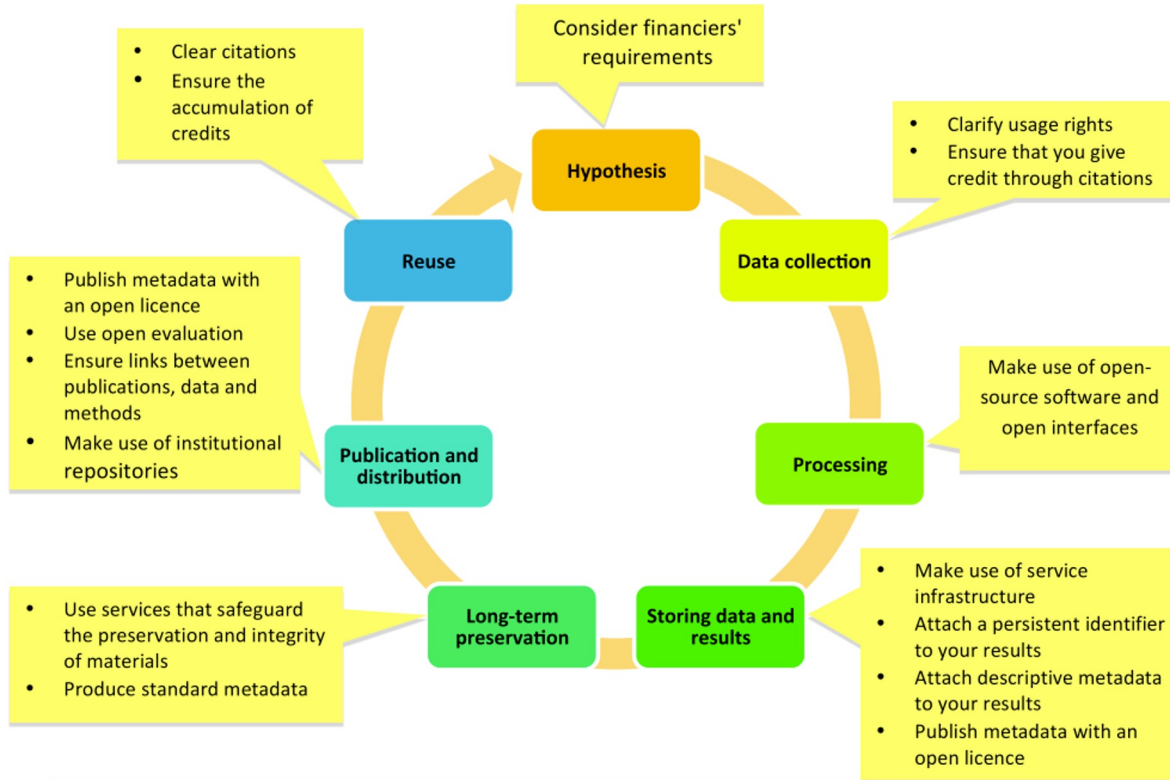
# What is OpenScience?

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



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

go-fair.org/fair-principles/



[FAIR Principles](#) [Implementation Networks](#) [News](#) [Events](#) [Resources](#) [About GO FAIR](#) [Q](#)

## FAIR Principles

[Home](#) > [FAIR Principles](#)

- > **FAIR Principles**
- > **F1: (Meta) data are assigned globally unique and persistent identifiers**
- > **F2: Data are described with rich metadata**
- > **F3: Metadata clearly and**

In 2016, the '[FAIR Guiding Principles for scientific data management and stewardship](#)' were published in *Scientific Data*. The authors intended to provide guidelines to improve the **F**indability, **A**ccessibility, **I**nteroperability, and **R**euse of digital assets. The principles emphasise machine-actionability (i.e., the capacity of computational systems to find, access, interoperate, and reuse data with none or minimal human intervention) because humans increasingly rely on computational support to deal with data as a result of the increase in volume, complexity, and creation speed of data.

A practical "how to" guidance to go FAIR can be found in the [Three-point FAIRification](#)

# OpenScience Taxonomy

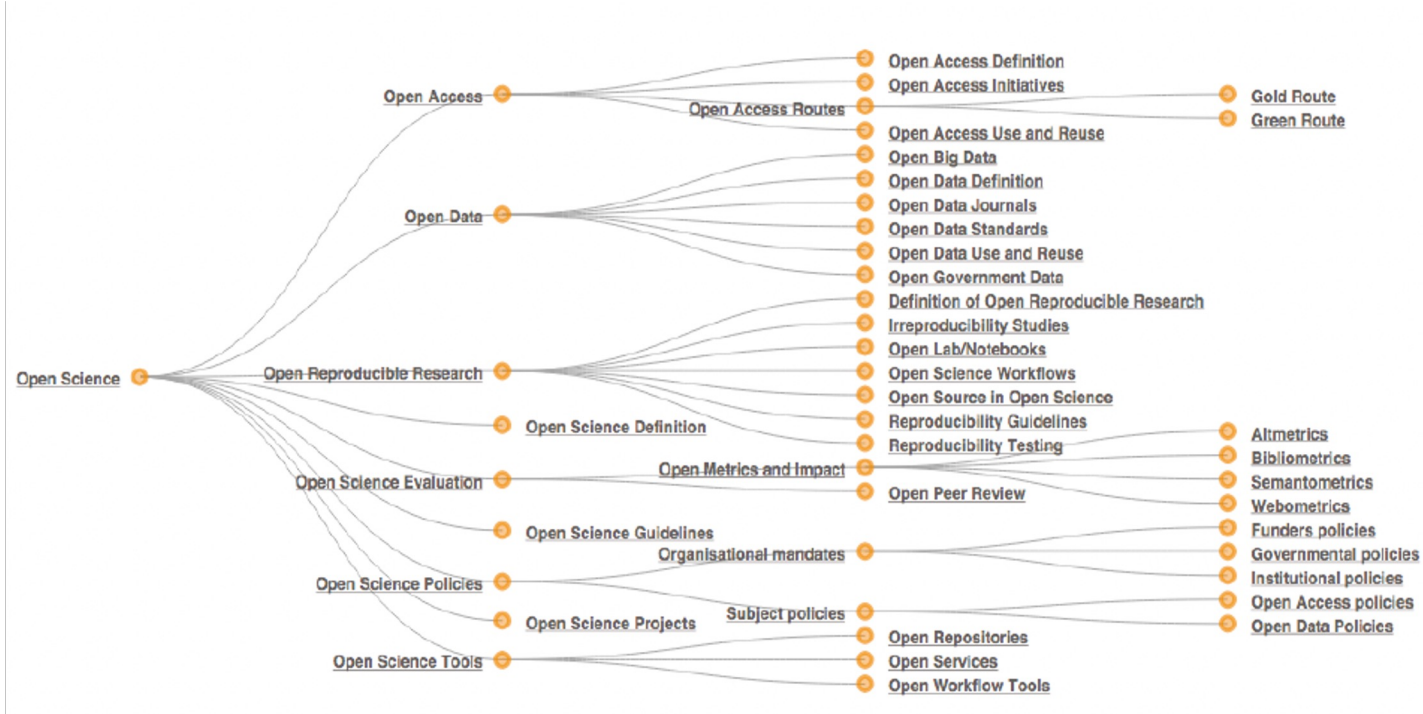


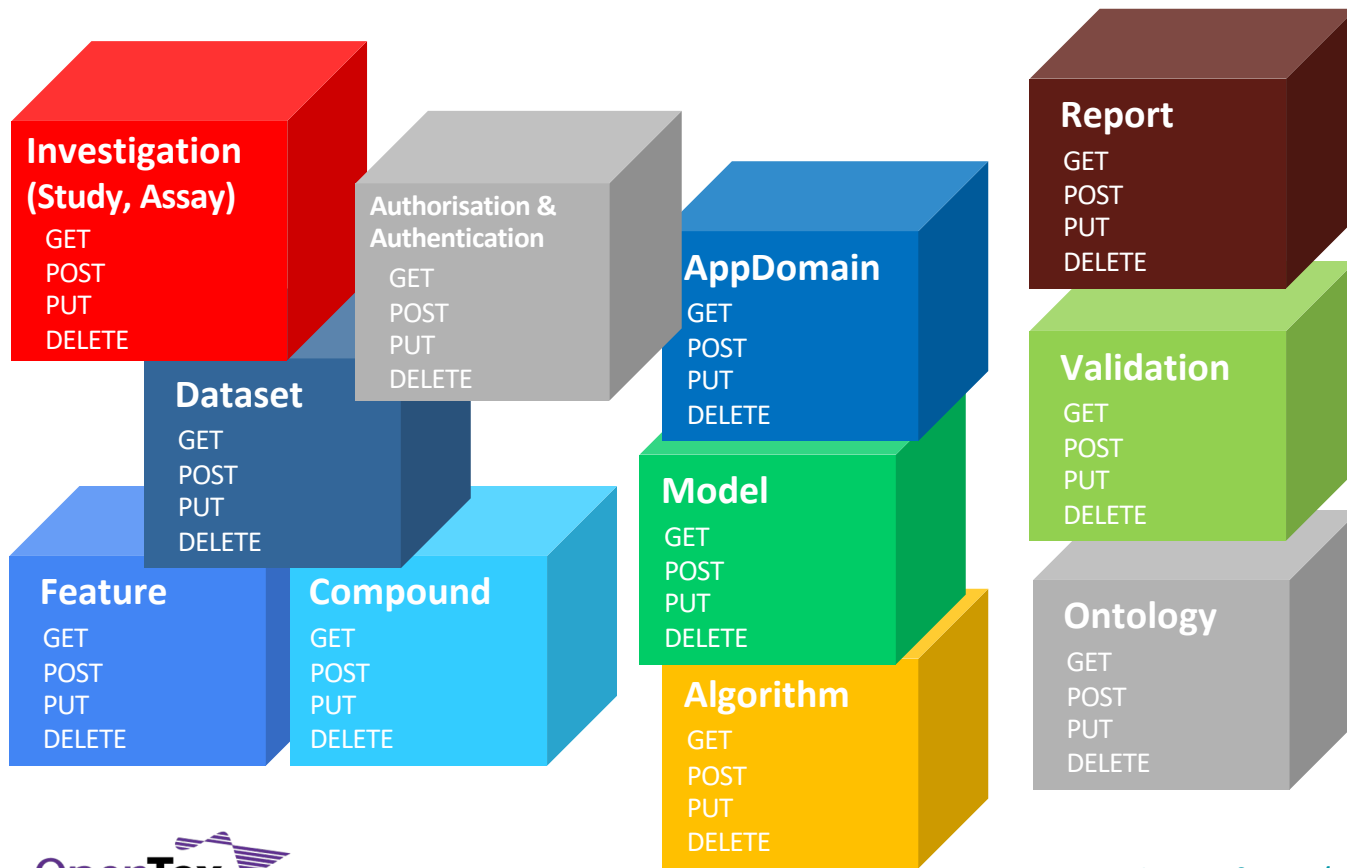
Image source: [Pontika et al., 2015](#)

# 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)



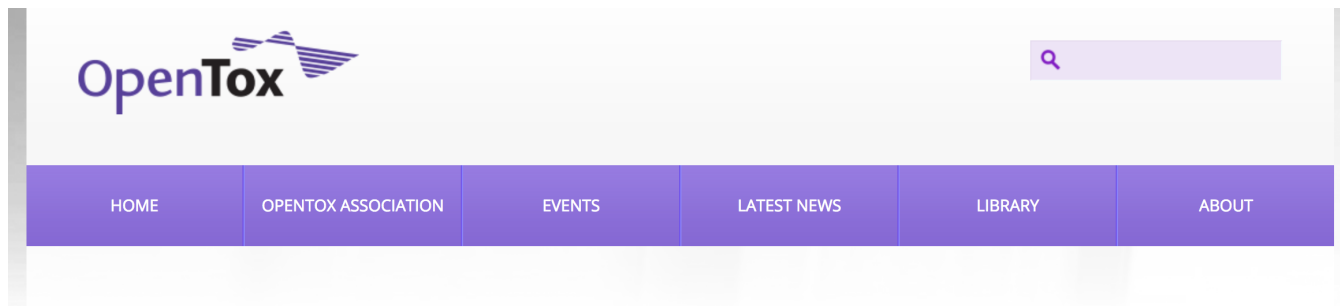
# Consensus on need for Common Language and Ontology



- 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](http://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 Jeliaskova (Ideacon), 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



## INTERNSHIP

### OPENTOX INTERNSHIP PROGRAM

The goals of the OpenTox Internship Program are:

1. To support work that progresses the goals of OpenTox
2. To support the career development of interns
3. To encourage knowledge development, sharing, and interaction

The projects should be small and focused in nature e.g., develop a case study, carry out a data analysis for the case study, lead the study in an OpenTox Hackathon etc. We anticipate that the work and related interactions can primarily be carried out virtually. Additionally, we can also consider traveling e.g., to visit an OpenTox member, work with their group, participate in a local hackathon.

## OPENTOX INTERNSHIP PROGRAM

- ▶ [ABOUT OPENTOX INTERNSHIP PROGRAM](#)
- ▶ [>> APPLY FOR INTERNSHIP <<](#)
- ▶ [DOWNLOAD INTERNSHIP REQUIREMENTS](#)

# OpenRiskNet – Integrated services and use cases

OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE

e-Infrastructure

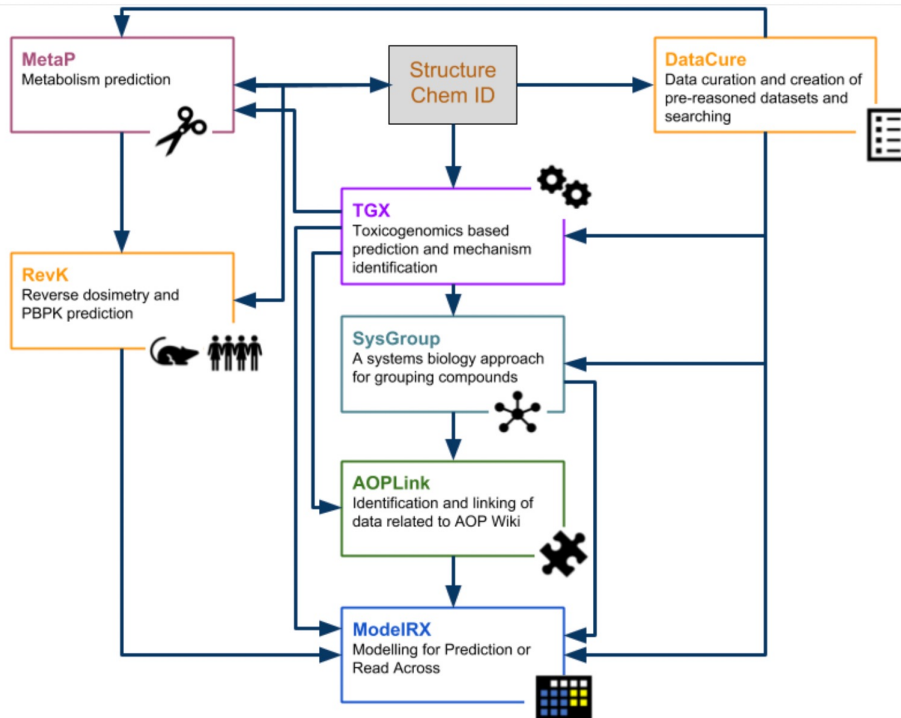
Resources & Training

Participate

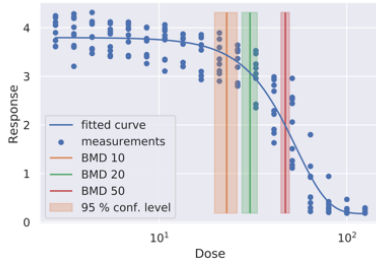
Events

News

About

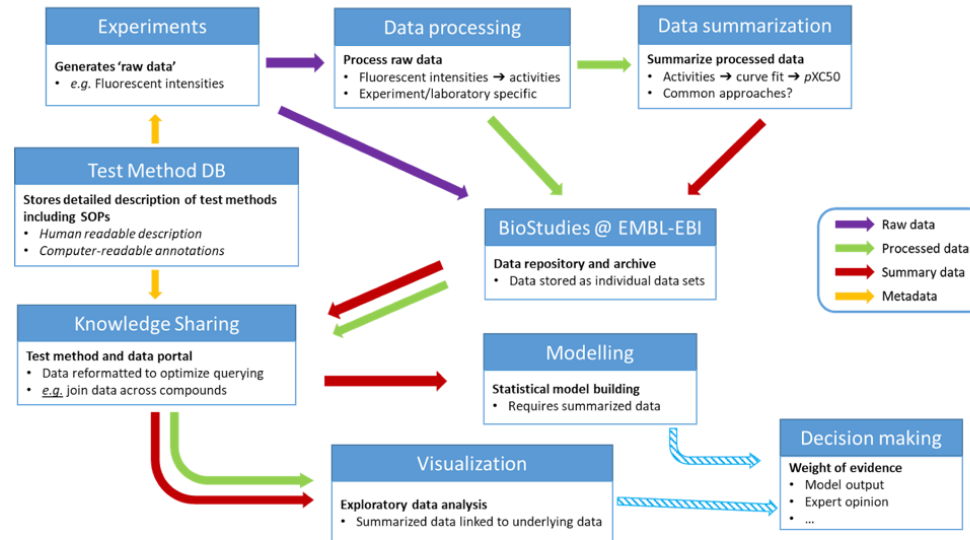


# Knowledge Management on EU-ToxRisk



Harmonised Data,  
Protocol and Metadata  
Management  
Infrastructure supported  
by EdelweissData

## Data and Knowledge Management on EUToxRisk program



# Data Generation template

## EU-ToxRisk data template

### Study

#### Search attributes:

- Data type
- Organ
- Organism
- Toxicity domain
- Compound
- Method name
- Project part

Links to related datasets

Contact information

### Compound info

#### Compound list with attributes:

- SMILES
- InChI key
- CAS #
- ...

### “Constant” and “variable” sheets

Sample

- ...

Assay

- ...

Compound

- Dosage scheme  
...

Sample grouping info

Endpoint definitions and data

Data file  
(.csv, fastq,  
etc)



# RISK-HUNT3R (2021 – 2026)

← → ↻ risk-hunt3r.eu

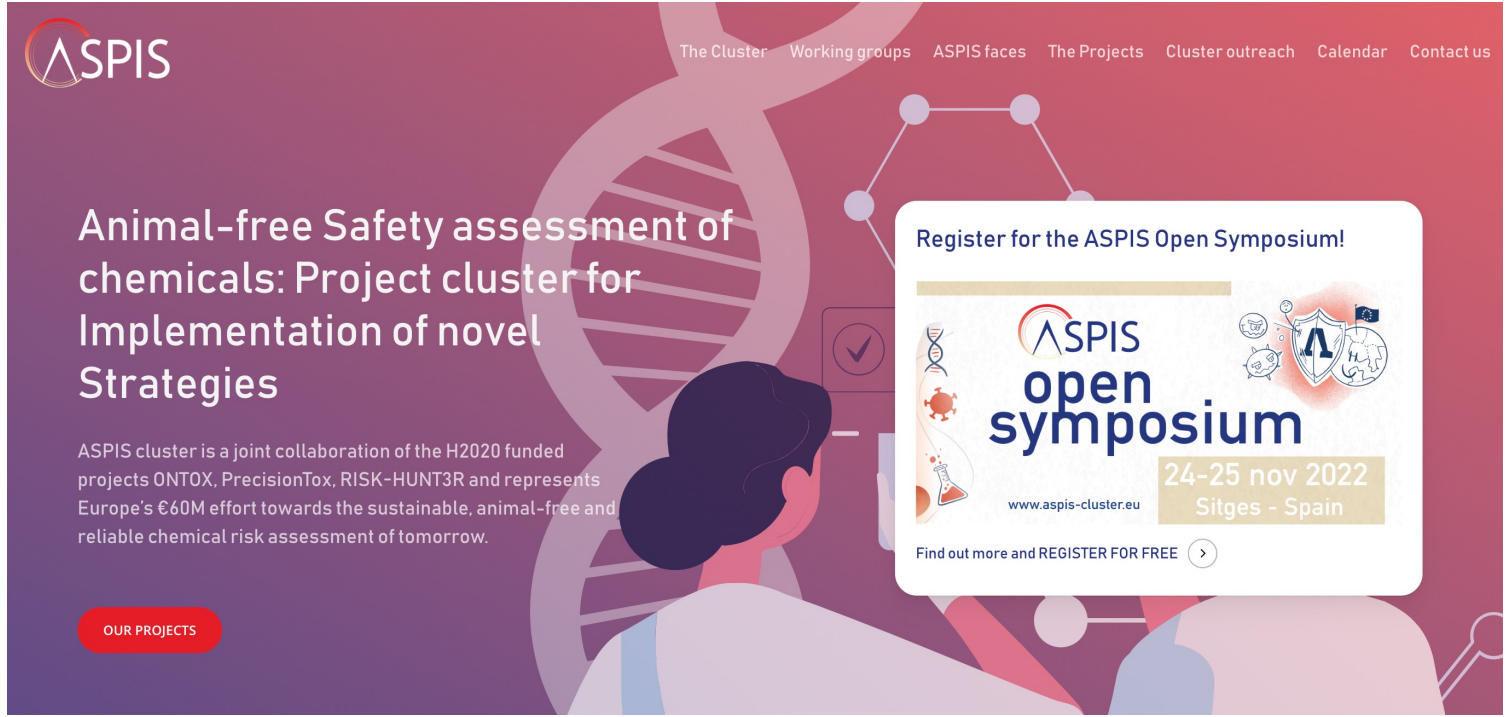
**RISK HUNT3R**

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**RISK-HUNT3R**  
RISK assessment of chemicals integrating HUMAN centric Next generation Testing strategies promoting the 3Rs

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



**ASPIS**


The Cluster Working groups ASPIS faces The Projects Cluster outreach Calendar Contact us

## Animal-free Safety assessment of chemicals: Project cluster for Implementation of novel Strategies

ASPIS cluster is a joint collaboration of the H2020 funded projects ONTOX, PrecisionTox, RISK-HUNT3R and represents Europe's €60M effort towards the sustainable, animal-free and reliable chemical risk assessment of tomorrow.

**OUR PROJECTS**

Register for the ASPIS Open Symposium!



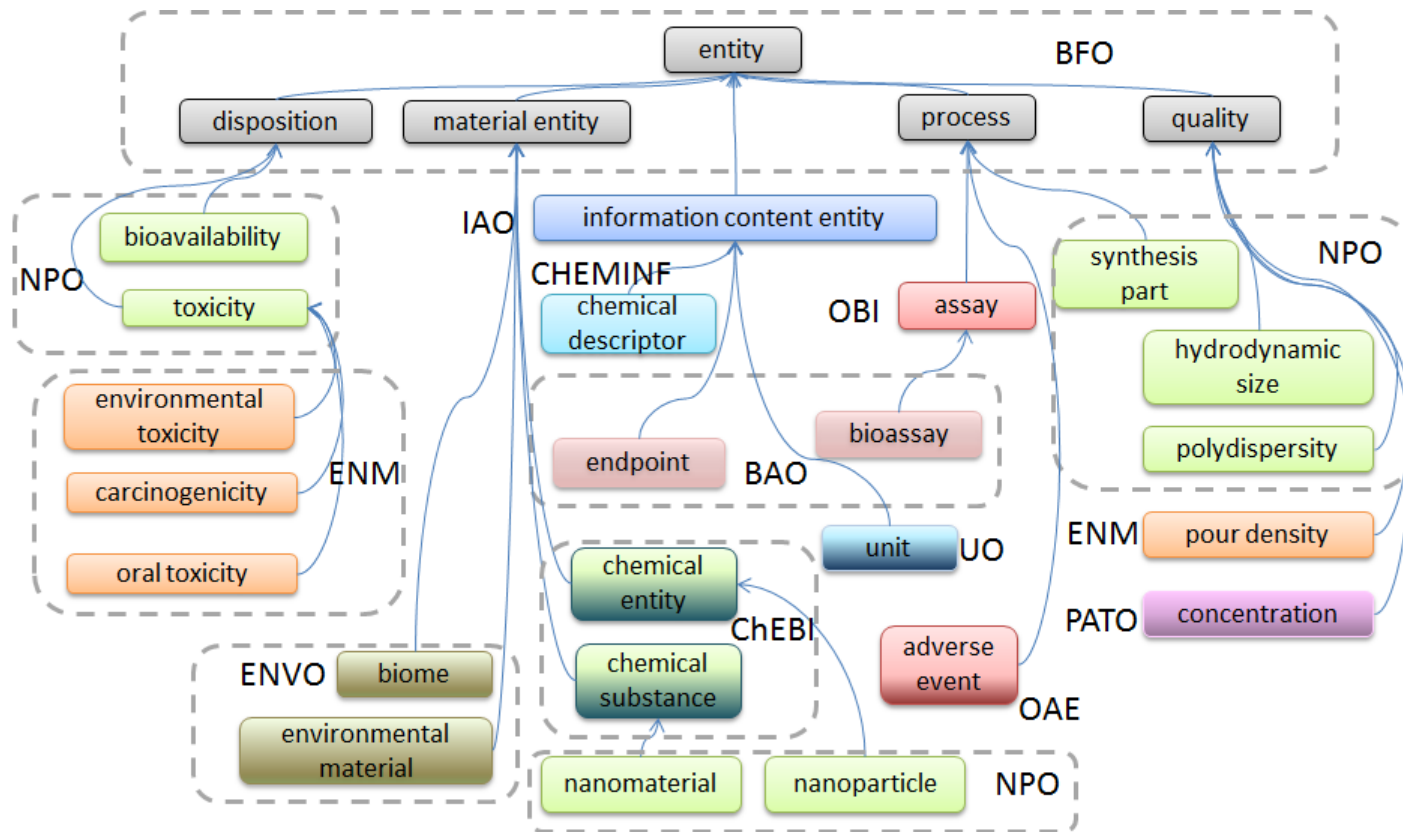
**ASPIS**  
**open symposium**

24-25 nov 2022  
Sitges - Spain

[www.aspis-cluster.eu](http://www.aspis-cluster.eu)

Find out more and REGISTER FOR FREE >

# ENanoMapper Ontology

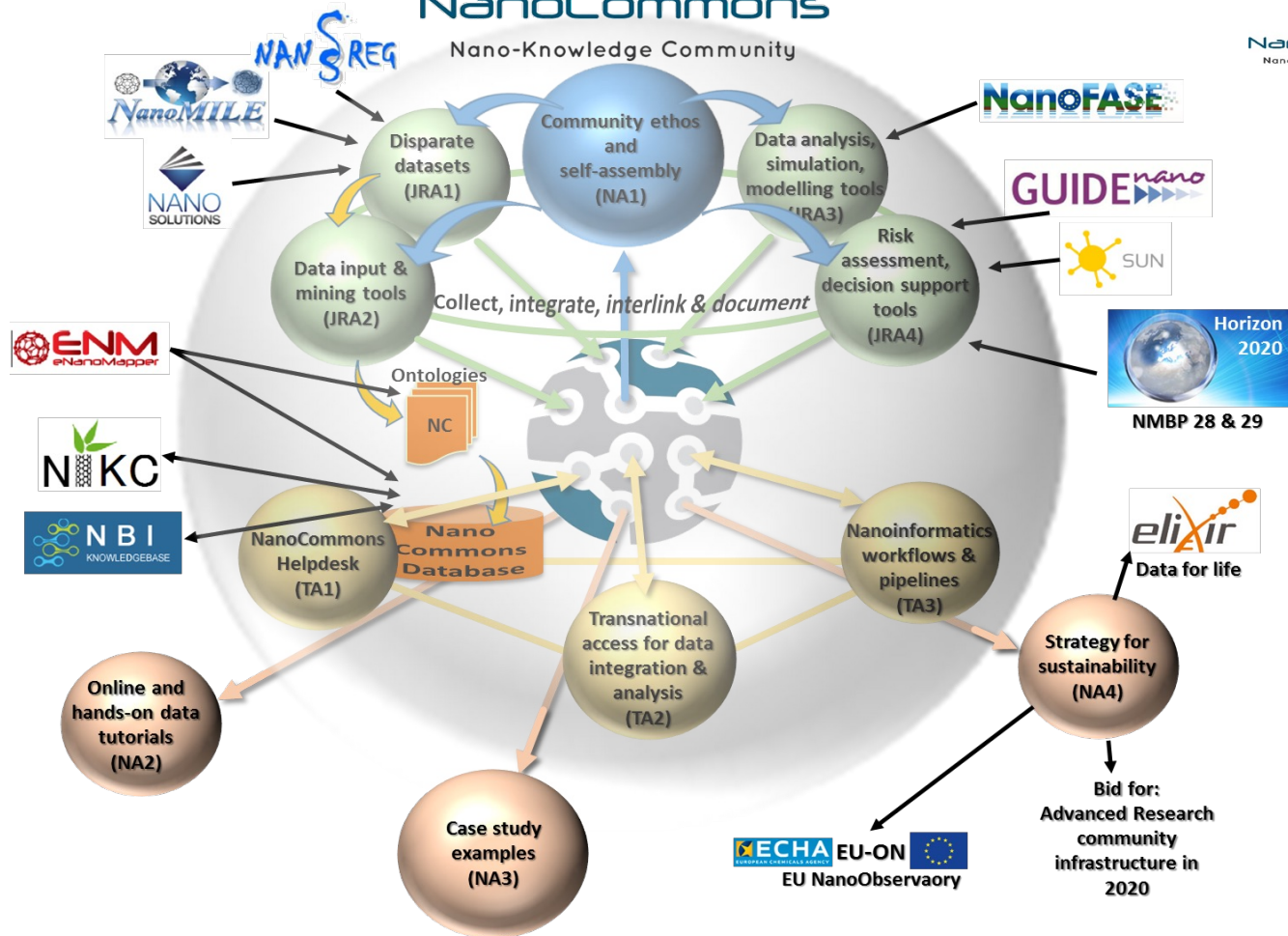




NanoCommons  
Nano-Knowledge Community

# NanoCommons

Nano-Knowledge Community



# AceNano Characterisation Infrastructure



[About ACEnano](#)

[ACEnano Team](#)

[News/Events](#)

[Contact us](#)

[Private area](#)

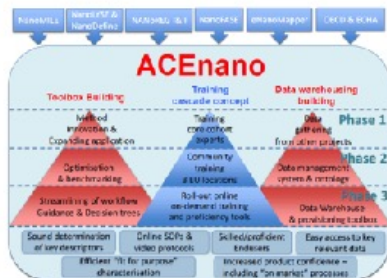
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Analytical and Characterisation Excellence in nanomaterial risk assessment: A tiered Approach

## ACEnano in a nutshell

ACEnano will introduce confidence, adaptability and clarity into nanomaterial risk assessment by developing a widely implementable and robust tiered approach to nanomaterial physicochemical characterisation that will simplify and facilitate contextual (hazard or exposure) description and its transcription into a reliable nanomaterials grouping framework.



This will be achieved by the creation of a "conceptual toolbox" including a tiered approach to cost-efficient nanomaterials analysis that will facilitate decision-making in choice of techniques and SOPs, linked to a characterisation methodology framework for grouping and risk assessment.

ACEnano will initiate activities to support data collection, management, interpretation and delivery to a data warehouse for safe use & storage. It will thus underpin the future of nanomaterial quality control, labelling and on-counterfeiting.

continuous training

## Next Events

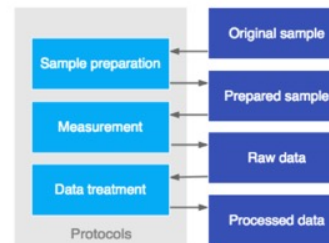
Week: 2317						
1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18	19	20	21
22	23	24	25	26	27	28



# Protocol Management

## ACEnano Protocols

The ACEnano Knowledge Infrastructure facilitates access and sharing of methodology applied in nanosafety, starting with nanomaterials characterisation protocols developed or optimised within the ACEnano project. The experimental datasets of nanomaterials characterization will be stored together with relevant metadata pertaining to sample preparation, the measurement, and the data treatment. The resulting measured value and its metadata will give as complete information as possible so that possibilities of future use of the measured value is maximised.



[Add a new protocol >](#)

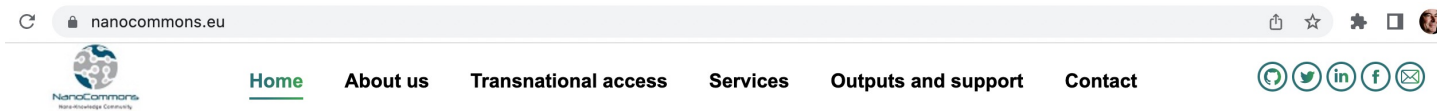
[My protocols >](#)

Enter keywords

Protocol type  Technique  Endpoint  Development phase  Organisation

Protocol type	Protocol	Posted
Data treatment	<b>HIC chromatogram analysis - v1_b</b> Analysis of HIC chromatograms	8 Apr 2021

# NanoCommons Knowledge Hub



## We develop, you access



### Experimental Workflows Design & Implementation

Automated data acquisition, online lab-books, data curation templates, nanoinformatics implementation.



### Data Processing & Analysis

From data cleansing, mining and analysis to modelling and from ISA-TAB tools to ontologies.



### Data Visualisation & Predictive Toxicity

Omics, QSARs, modelling and risk assessment tools.



### Data Storage & Online Accessibility

Data repositories, storage, online access

<https://www.nanocommons.eu/>

# NanoCommons User guidance handbook

Q Search NanoMaterialCommons User Handbook

Data management / Nanosafety data resources

## Listing of important data resources for nanosafety and nanoinformatics

### ACEnano knowledge warehouse

Specializing on physico-chemical characterisation techniques, protocols and data.

### NanoCommons knowledge base and data warehouse

One-stop shop for nanosafety data by linking in different data warehouses and also the primary home of data from different projects including NanoMile, NanoFASE and SmartNanoTox.

### Nanosafety data interface

Home of data from many projects. Currently, eNanoMapper, NANoREG and NanoReg2 are publicly available.

### CEINT Nanoinformatics Knowledge Commons (NIKC)

Literature curated data describing nanomaterials in terms of their intrinsic, extrinsic (system-dependent), and social (e.g. anticipated use scenarios, matrix, concentration in products) properties, system characteristics (environmental, biological, laboratory, etc.), exposure and hazard measurements, calculations, and estimates.

### Nanomaterial-biological interactions knowledgebase

Repository for annotated data on nanomaterial characterization (purity, size, shape, charge, composition, functionalization, agglomeration state), synthesis methods, and nanomaterial-biological interactions (beneficial, benign or deleterious) defined at multiple levels of biological organization (molecular, cellular, organismal)

Powered by NanoCommons and Seven Past Nine and based on Jekyll and Just the Docs.

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Edit this page on GitHub.



Q Search NanoMaterialCommons User Handbook

Q Search NanoMaterialCommons User Handbook

Data management / Nanosafety data resources / ACEnano Knowledge Infrastructure

## NanoCommons Knowledge Infrastructure



This page provides information on the Knowledge Infrastructure of the ACEnano Project - Analytical and Characterisation Excellence in nanomaterial risk assessment: a tiered approach.

ACEnano aimed to introduce confidence, adaptability and clarity by providing a widely implementable and robust tiered approach to nanomaterials physicochemical characterisation that simplifies and facilitates contextual (hazard or exposure) description and its transcription into a reliable nanomaterials grouping framework.

To be able to

1. NanoCommons

NanoCommons

interfaces

2. NanoCommons

made public

For the data

and browsed

data provides

they want to

NanoCommons

### Access

 ACEnano knowledge warehouse

### Training

An overview of the functionalities of the knowledge warehouse was presented at an ACEnano workshop as part of the NanoTechnology conference. This covered the catalogue of techniques and endpoints, the protocol documentation concept and repository, and the data warehouse.

### Access

 NanoCommons

### Training

The session

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 ACEnano Knowledge Warehouse manual

 Slides from the NSC Week 2019 - Introduction

 Slides from the NSC Week 2019 - Training

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



openstack. Federated • VO:openrisknet.org

Project / Compute / Instances

## Instances

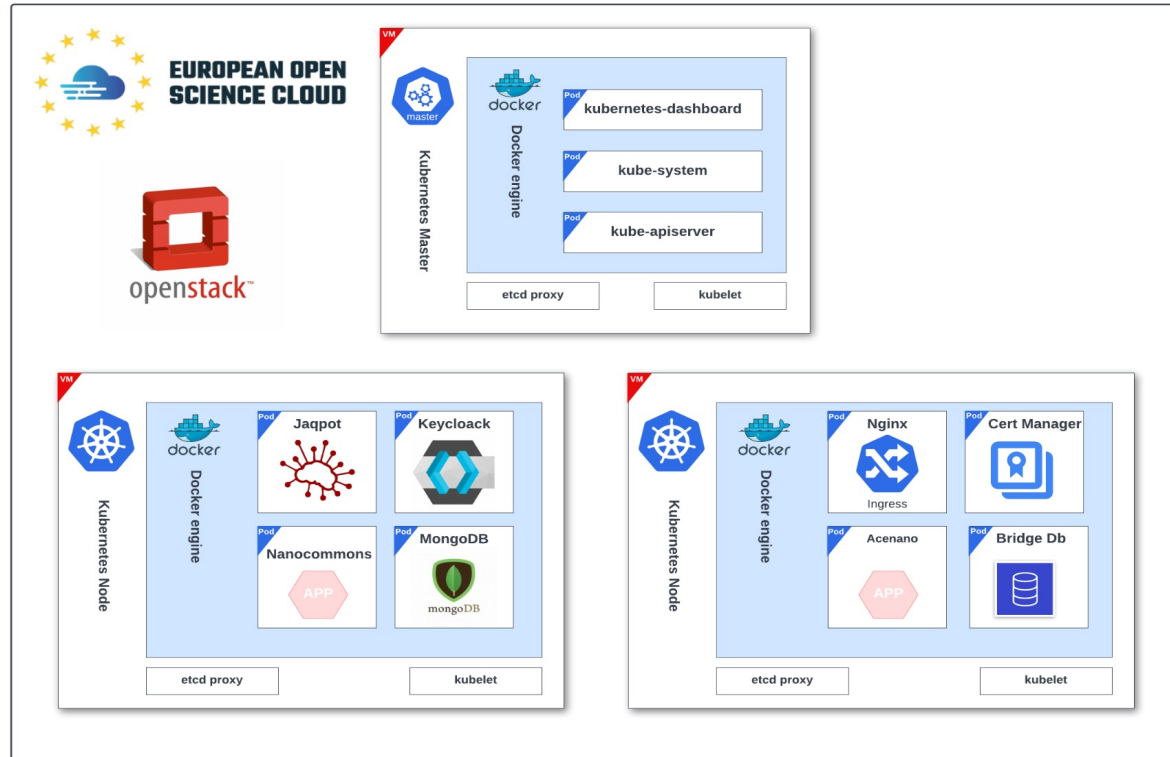
Instance ID =  Filter [Launch Instance](#) [Delete Instances](#) [More Actions](#)

Displaying 7 items

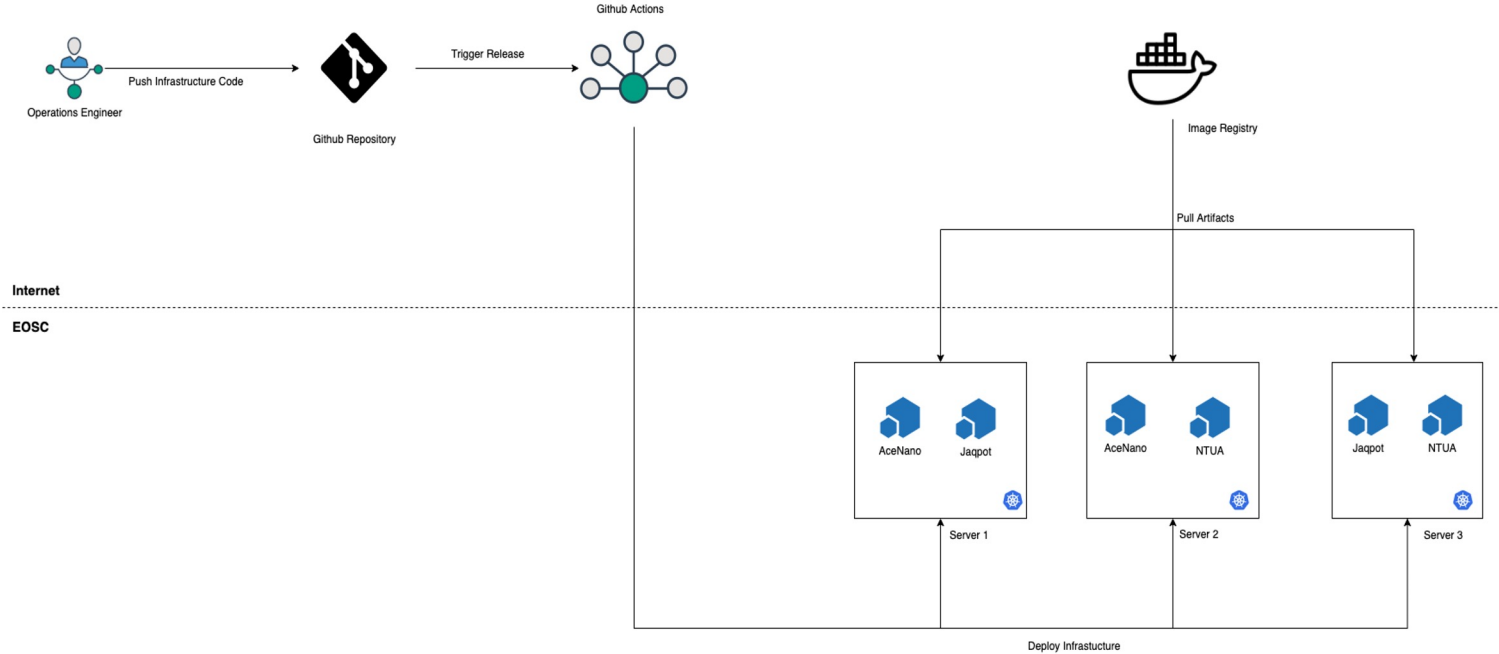
<input type="checkbox"/>	Instance Name	Image Name	IP Address	Flavor	Key Pair	Status	Availability Zone	Task	Power State	Age	Actions
<input type="checkbox"/>	Storage	IFCA Ubuntu 20.04 [2021-10-16]	172.16.95.22	cm4.large	eosc-cluster	Active	nova	None	Running	3 months, 2 weeks	<a href="#">Create Snapshot</a>
<input type="checkbox"/>	Master	IFCA Ubuntu 20.04 [2021-10-16]	172.16.95.3, 193.146.75.166	cm4.large	eosc-cluster	Active	nova	None	Running	3 months, 2 weeks	<a href="#">Create Snapshot</a>
<input type="checkbox"/>	Node-2	IFCA Ubuntu 20.04 [2021-10-16]	172.16.95.7	cm4.xlarge	eosc-cluster	Active	nova	None	Running	3 months, 2 weeks	<a href="#">Create Snapshot</a>
<input type="checkbox"/>	Node-3	IFCA Ubuntu 20.04 [2021-10-16]	172.16.95.34	cm4.xlarge	eosc-cluster	Active	nova	None	Running	3 months, 2 weeks	<a href="#">Create Snapshot</a>
<input type="checkbox"/>	Node-1	IFCA Ubuntu 20.04 [2021-10-16]	172.16.95.15	cm4.xlarge	eosc-cluster	Active	nova	None	Running	3 months, 2 weeks	<a href="#">Create Snapshot</a>
<input type="checkbox"/>	ingress	IFCA Ubuntu 20.04 [2021-10-16]	172.16.95.8	cm4.large	eosc-cluster	Active	nova	None	Running	3 months, 2 weeks	<a href="#">Create Snapshot</a>
<input type="checkbox"/>	mant	IFCA Ubuntu 20.04 [2021-10-16]	172.16.95.21	m1.small	eosc-	Active	nova	None	Running	4 months	<a href="#">Create Snapshot</a>

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

Interest in Knowledge Infrastructure Participation Form:

<https://forms.gle/bNCqZqu8Ln2pFnMk9>