



**NanoCommons**

Nano-Knowledge Community

# **The European Nanotechnology Community Informatics Platform: Bridging data and disciplinary gaps for industry and regulators**



This project has received funding from the European Union Horizon 2020  
Programme (H2020) under grant agreement no. 731032



**NanoCommons**

Nano-Knowledge Community

**The NanoCommons knowledge infrastructure  
built to support the research communities, industrial users and  
regulators in the area of nanomaterials safety assessment**

**Thomas Exner - Edelweiss Connect**

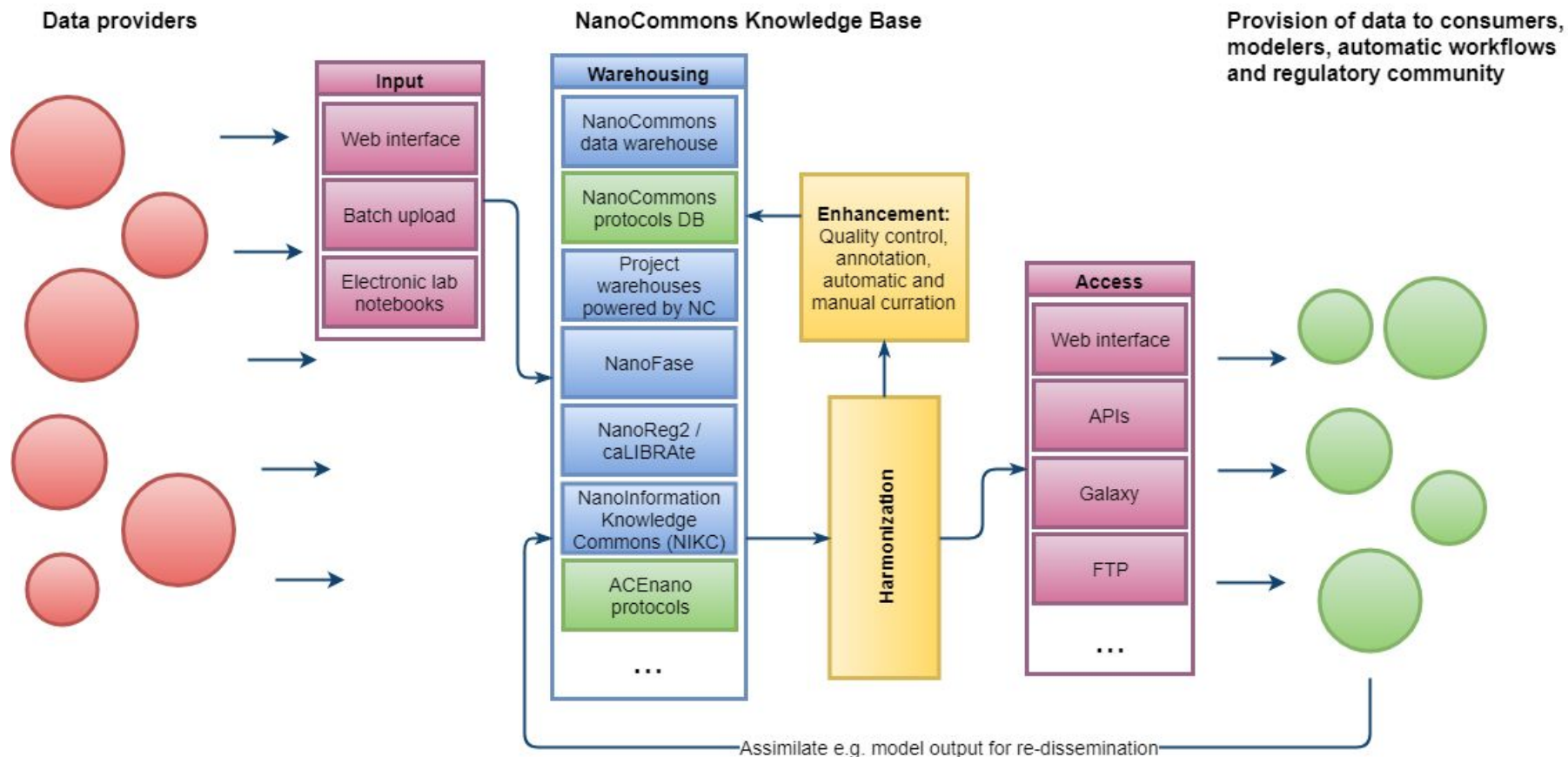
***NanoSafety Cluster week  
Copenhagen, 9 October 2019***

# Data Driven Innovation – Added Value

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# Scope of the data management tasks



# Data management and sharing

# NanoCommons Knowledge Infrastructure






NanoCommons Platform

[Home](#)
[News](#)
[My Profile](#)
[Help](#)
[Help Desk](#)
[Analysis](#)
[Browse Ontologies](#)
[Data Access](#)
[Data Upload](#)


BioXNA

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Welcome to the NanoCommons Knowledge Base




Analysis



Data Access

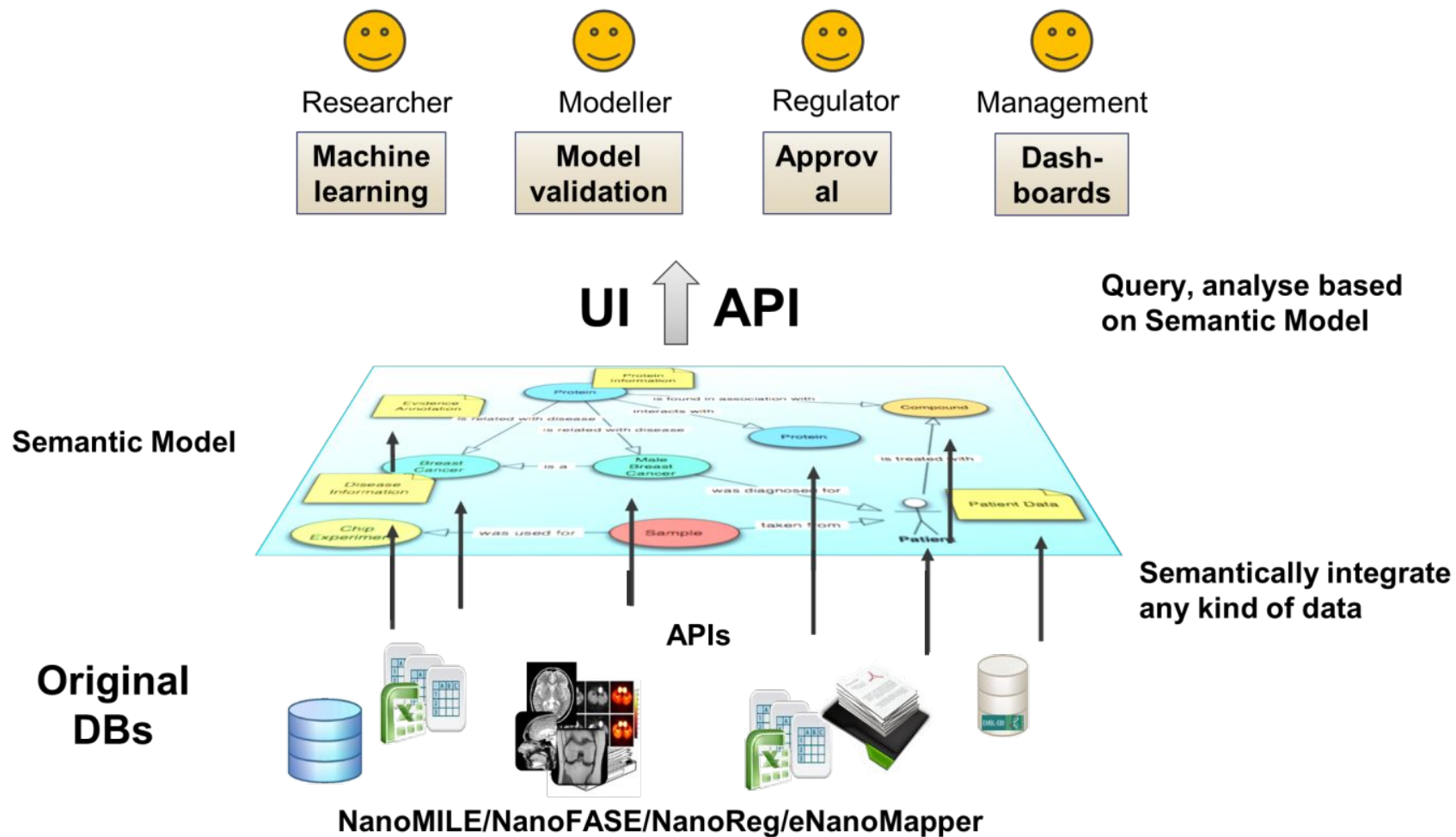


Upload Data



Ontologies

# Why is it more than data warehousing?





# NanoCommons data warehouse



NanoCommons Platform

Search...



Home



News



My Profile



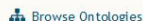
Help



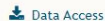
Help Desk



Analysis



Browse Ontologies



Data Access



Data Upload

BioXM » Particles

Export

Folder

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Admin



## Particle Characterisation

Characterisation data

ID



Search

+ Add

Selected items: 0

Show/Hide

Sort by

Further Information

ID	Chemical Elements	Characterisation data	Samples	Aliquots	NanoFASE name	Designator
NP00190	Ce	NP00190	SIGMA-CeO2Bulk-5microns-030314 SIGMA-CeO2Bulk-5microns-230114 SIGMA-CeO2Bulk-5microns-300114	SIGMA-CeO2Bulk-5microns-030314b SIGMA-CeO2Bulk-5microns-230114a SIGMA-CeO2Bulk-5microns-300114a		
NP00191	Ce	NP00191	JRC-CeO2-NM02101a002230	JRC-CeO2-NM211-2163a		

View: General - NanoFASE - Instance

Manage...

ID	Name	Instance ID	Time of Measure...	Time of Measur...	Medium	Sample	Protocol ID	Name	Description	Step	Step.St...	Step.Name	Step.De...
IN000011702	01.001/1000_stock dispersion	stock dispersion	0.0 min	0.0 min		SAMP_000000463 MWCNT powder SAMP_000000472 MWCNT powder							
IN000011703	01.001/1000_control	control	0.0 min	0.0 min	Leached solution	SAMP_000000464 Released materials SAMP_000000473 Released materials							
IN000011704	01.001/1000_I0	10	0.0 min	0.0 min	Plastic product	SAMP_000000465 MWCNT-PP SAMP_000000474 MWCNT-PP	01.001/1000_3 01.001/1000_6	SEM-EDX analysis Nanocomposite	ISM-6010 LV, JEOL Ltd. (CoolSafe 100-9 PRO				
IN000011705	01.001/1000_I2	12	200.0 min	200.0 min	Aged plastic product	SAMP_000000466 Aged MWCNT-PP SAMP_000000475 Aged MWCNT-PP	01.001/1000_4 01.001/1000_6 01.001/1000_7	Weathering 200 h Nanocomposite recycling	(CoolSafe 100-9 PRO	01.001/1000_1.0		Climatic	climatic
IN000011706	01.001/1000_I3	13	0.0 min	200.0 min	Powder of aged plastic product	SAMP_000000467 Milled aged MWCNT-PP SAMP_000000476 Milled aged MWCNT-PP							
IN000011707	01.001/1000_I4	14	0.0 min	200.0 min	Recycled Plastic product	SAMP_000000468 Recycled MWCNT-PP SAMP_000000477 Recycled MWCNT-PP	01.001/1000_3 01.001/1000_4 01.001/1000_6 01.001/1000_7	SEM-EDX analysis Weathering 200 h Nanocomposite recycling	ISM-6010 LV, JEOL Ltd. (CoolSafe 100-9 PRO	01.001/1000_1.0		Climatic	climatic
IN000011708	01.001/1000_I5	15	1000.0 min	1200.0 min	Weathered Recycled Plastic product	SAMP_000000469 Weathered recycled MWCNT-PP SAMP_000000478 Weathered recycled MWCNT-PP	01.001/1000_3 01.001/1000_4 01.001/1000_5	SEM-EDX analysis Weathering 200 h Weathering 1000 h	ISM-6010 LV, JEOL Ltd.	01.001/1000_1.0		Climatic	climatic
IN000011709	01.001/1000_I6	16	0.0 min	1200.0 min	Leached solution	SAMP_000000479							
IN000011710	01.001/1000_I7	17	0.0 min	1200.0 min	Leached solution	SAMP_000000480							

View: General - Instrument

Manage...

Instrument

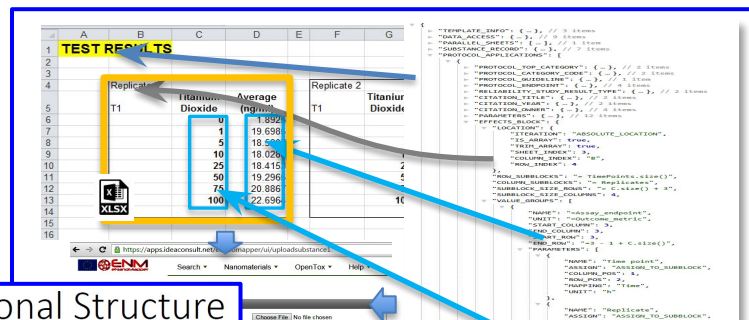


Search

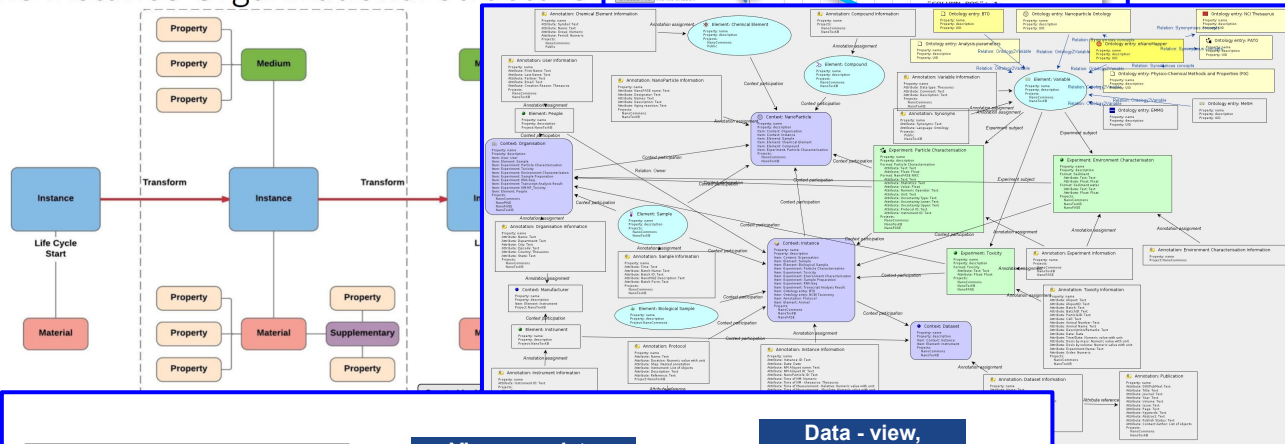
Instrument	Manufacturer	Used for dataset
● IEM-2100	● JEOL	● 01.001/1000
● D5000	● Bruker	● 01.001/1000
● Agilent 7500	● Agilent Technologies	● 01.001/1000
● CEM 1600W	● MARS	● 01.001/1000
● NR50 E	● OVAN	● 01.001/1000
● 6500F FEG-SEM	● JEOL	● 01.001/1000
● TGA Q500	● TA instruments	● 01.001/1000
● Suntest XXL+	● Atlas	● 01.001/1000
● extruder TSE20	● Brabender	● 01.001/1000
● mDSC_Q20	● TA instruments	● 01.001/1000
● Affinity-L 8400	● Shimadzu	● 01.001/1000
● ISM-6010 LV	● JEOL	● 01.001/1000



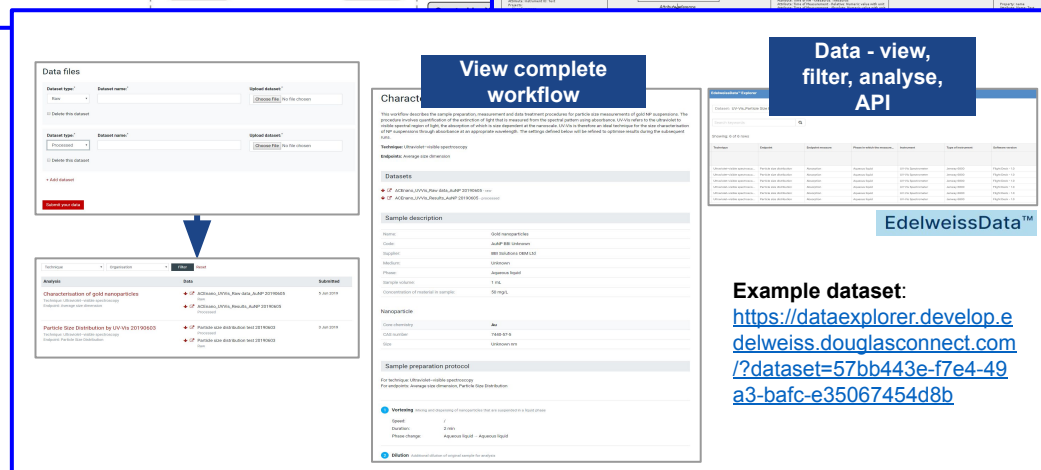
- eNanoMapper



## NIKC Instance Organizational Structure



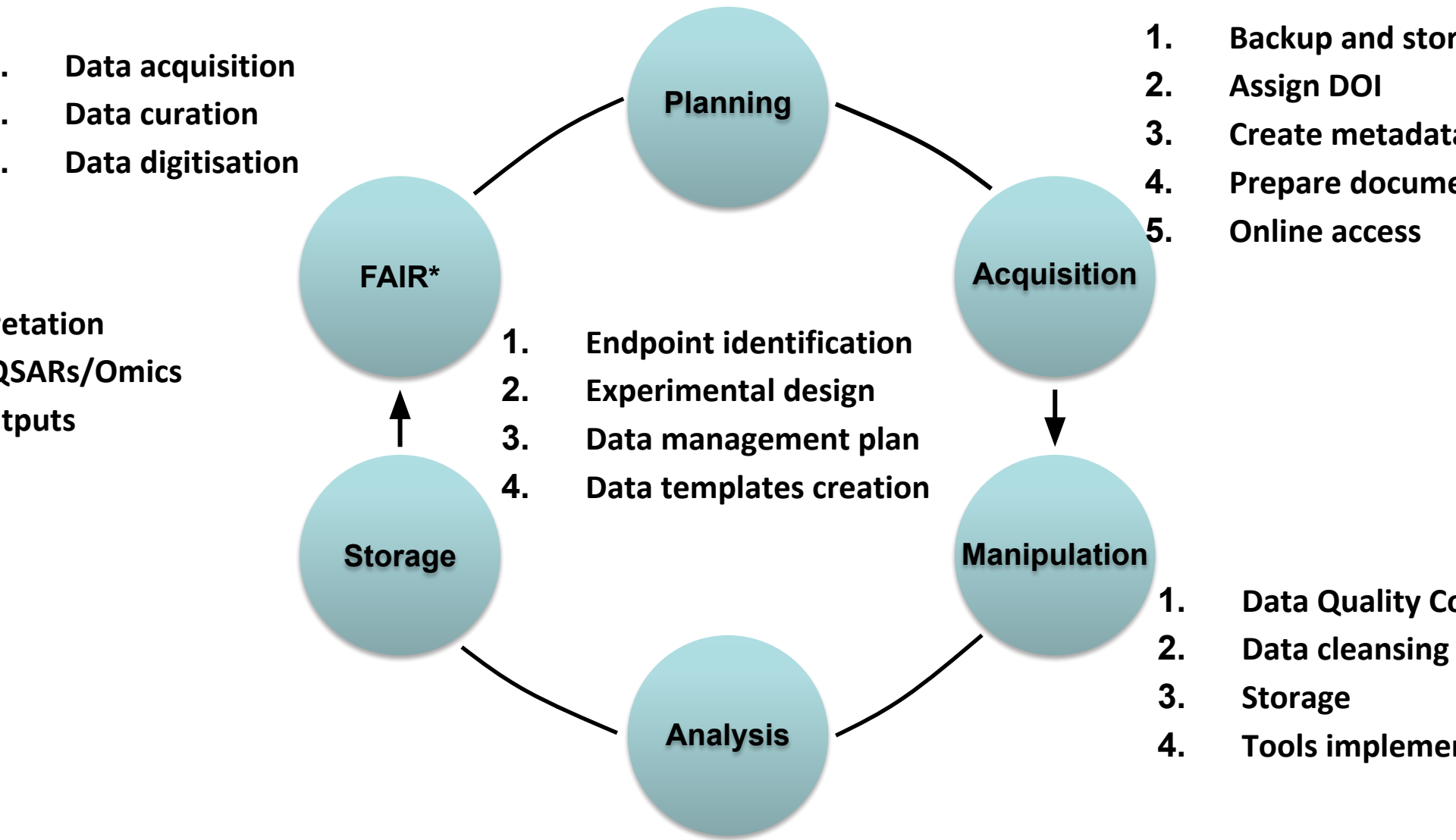
- ACEnano



**Example dataset:**  
<https://dataexplorer.develop.edelweiss.douglasconnect.com/?dataset=57bb443e-f7e4-49a3-bafc-e35067454d8b>

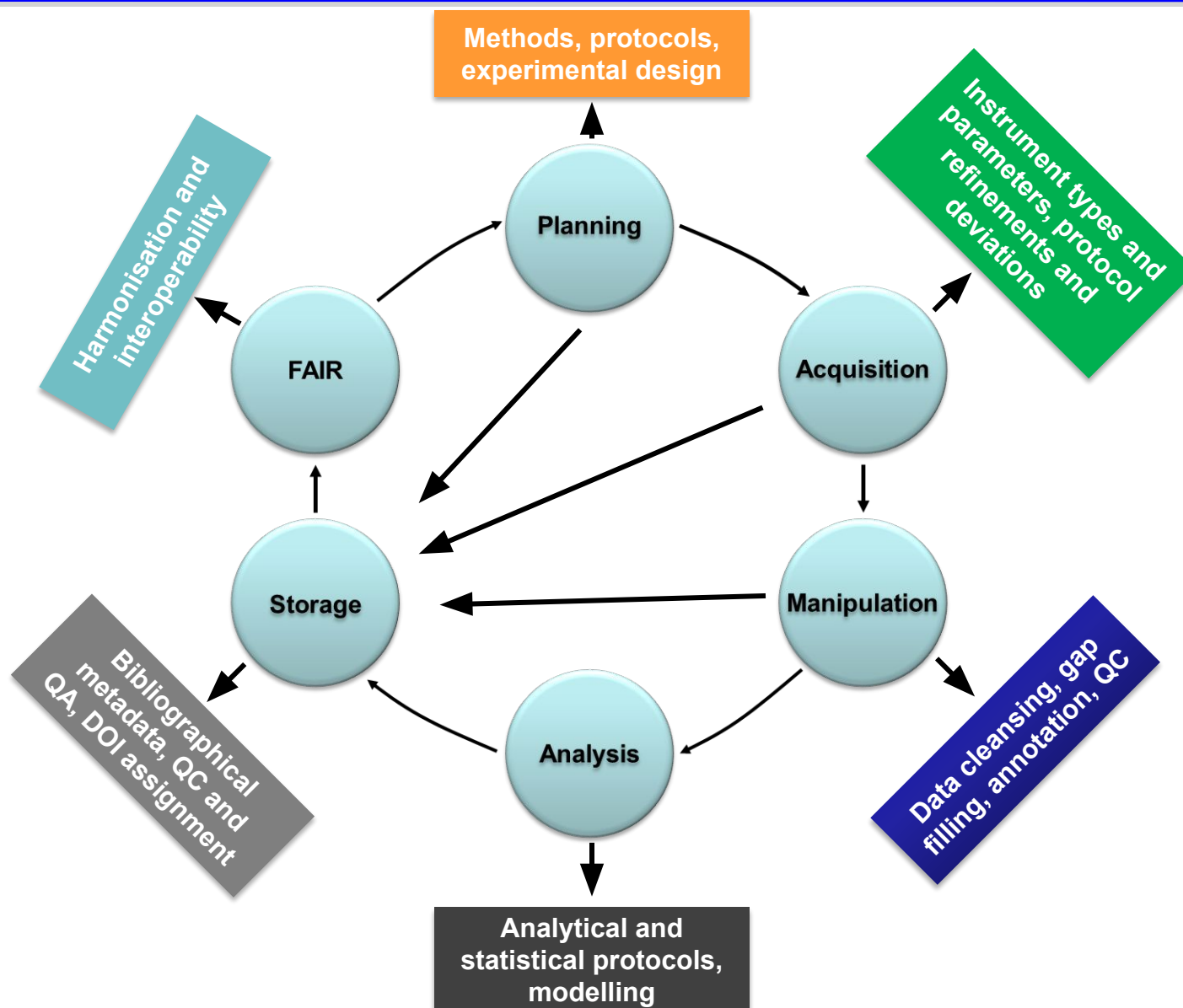
# Data quality

# Data management and data lifecycle



\*Findable, Accessible, Interoperable, Reusable

# Data management, data lifecycle & metadata



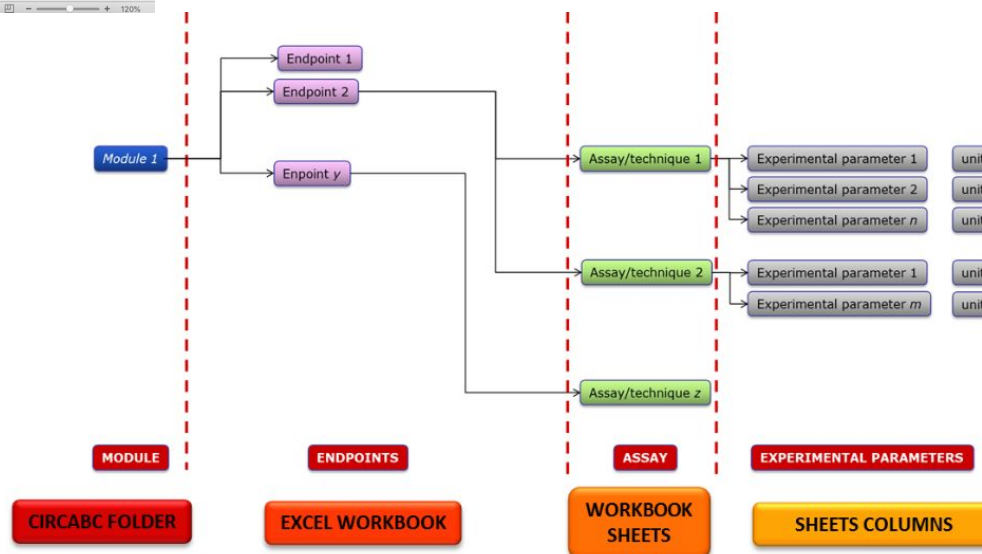
# Can we harmonize data capturing?

datasetid	Instance	Registry number	Material	Medium	measurementType	parameter	Inheritid	parameterDescription	parameterDataType	parameterText	parameterUnit
01.001/1000	Stock dispersion		Envirox CeO2 NP	Water	property	CeO2 concentration		Reported by Experimenter	numeric		mean
01.001/1000	Stock dispersion		Envirox CeO2 NP	Water	property	mean primary particle size		Reported by Experimenter	numeric		mean
01.001/1000	10		Sewage sludge	property	Ce concentration			Reported by Experimenter	numeric		mean
01.001/1000	10		Sewage sludge	property	Total solids			Reported by Experimenter	numeric		mean
01.001/1000	11		Sewage sludge	Property	Total solids			Reported by Experimenter	Numeric		
01.001/1000	11		Envirox CeO2 NP	Sewage sludge	Property	Amount		Reported by Experimenter	Numeric	Amount of Ce added to the sludge	
01.001/1000	12			Dry sewage sludge	property	Mass		Reported by Experimenter	numeric		
01.001/1000	12			Dry sewage sludge	property	Ce concentration		Reported by Experimenter	numeric		mean
01.001/1000	12			Dry sewage sludge	property	Ash content		Reported by Experimenter	numeric		
01.001/1000	12			Dry sewage sludge	Property	Total carbon		Reported by Experimenter	Numeric		
01.001/1000	12		Envirox CeO2 NP	Dry sewage sludge	property	XAS		Reported by Experimenter	numeric	Data at Eswag	
01.001/1000	13		Fly Ash	property	Mass			Reported by Experimenter	numeric		
01.001/1000	13		Fly Ash	property	Ce concentration			Reported by Experimenter	numeric		mean
01.001/1000	13		Fly Ash	Property	Total carbon			Reported by Experimenter	Numeric		
01.001/1000	13		Envirox CeO2 NP	Fly Ash	property	XAS		Reported by Experimenter	numeric	Data at Eswag	
01.001/1000	13		Envirox CeO2 NP	Fly Ash	property	TEM		Reported by Experimenter	numeric	Data at Eswag	
01.001/1000	14			Bottom ash	property	Mass		Reported by Experimenter	numeric		
01.001/1000	14			Bottom ash	property	Ce concentration		Reported by Experimenter	numeric		mean
01.001/1000	14			Bottom ash	Property	Total carbon		Reported by Experimenter	Numeric		
01.001/1000			SkySprings CeO2	Water	property	CeO2 concentration		Reported by Experimenter	numeric		mean
01.001/1000			SkySprings CeO2	Water	property	mean primary particle size		Reported by Experimenter	numeric		mean

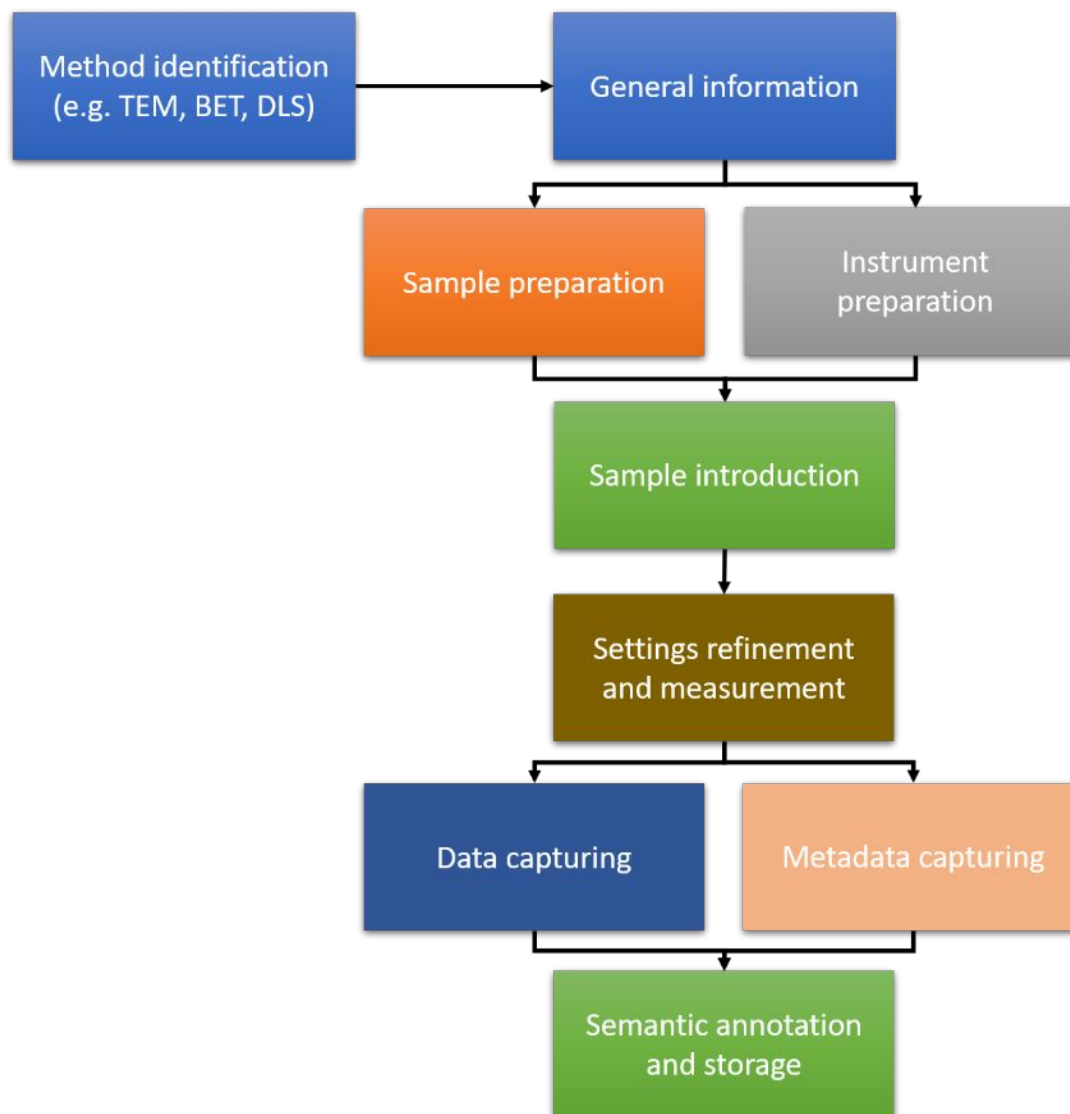
NIKC

- Evaluation of data capturing templates.

## NanoREG templates



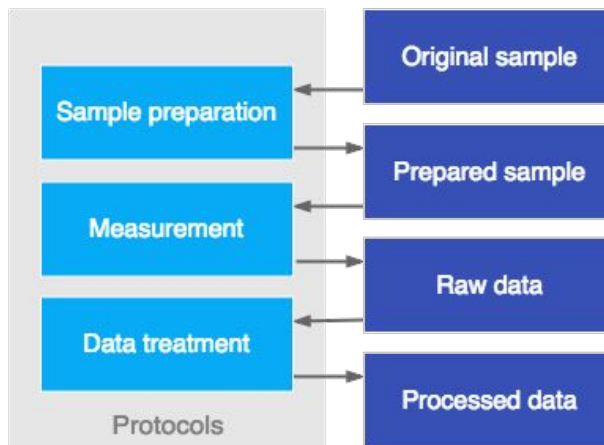
# Protocols capturing workflow





## Protocols

- Access and sharing of methods
- Collection of metadata on the experimental procedure
- Tracking details on the steps performed
- Linked the method with the result
- Comparison of the experimental design
- Searchable and easy to filter database



## Data

- Selection and use any of the methods added in the protocols database
- Create and save the full workflow applied
- Support intra- and inter-laboratory reproducibility goal
- Document all steps performed on a sample from the identification to the final characterisation results
- Storage and sharing of data



## Part 2: Equipment

### Equipment

Please describe the equipment used to perform the measurement. Be sure to provide details or may introduce artefacts in the final result.

**Name:\***  **Model:**  **Instrument type:**

Common instrument makes and models.

**Software:**  **Software version:**

**Limit of detection upper:**  **Limit of detection lower:**  **Limit of detection:**

What is the largest value of the endpoint that can be measured? If there are no definite detection limits please mention the particle or medium properties that limits the detectability as a function of size.

What is the lowest value of the endpoint that can be measured?

#### Instrument settings and parameters (optional)

List instrument settings and parameters that might influence the measured value or its accuracy, or are of importance for reproducing give units of these settings.

Setting	Value	Unit	<input type="checkbox"/> delete
Setting	Value	Unit	<input type="checkbox"/> delete
Setting	Value	Unit	<input type="checkbox"/> delete

### Possible datasets

State the type and units of each of the axes of raw data that can be produced by your instrument endpoint in question.

**Axe:\***  **Units:**  ☐ Delete

+ Add another axe

### Measurement quality parameters

State parameters that are measured by the instrument that give an indication of the accuracy or also their units if applicable.

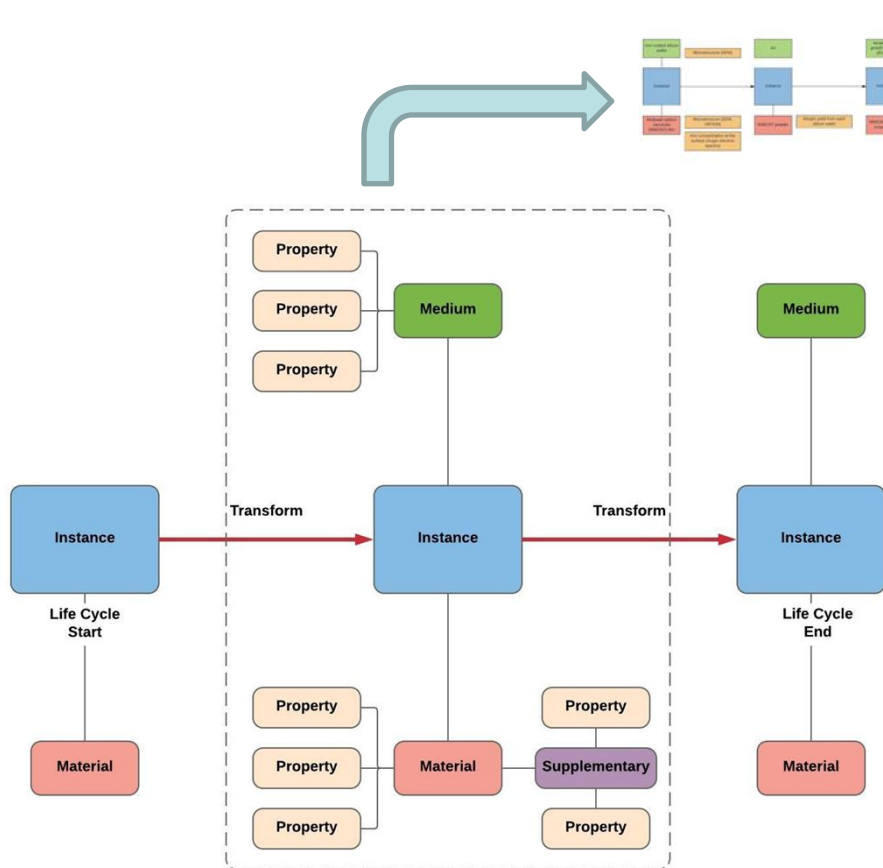
**Parameter:\***  **Common setting:**  **Units:**

+ Add another quality parameter

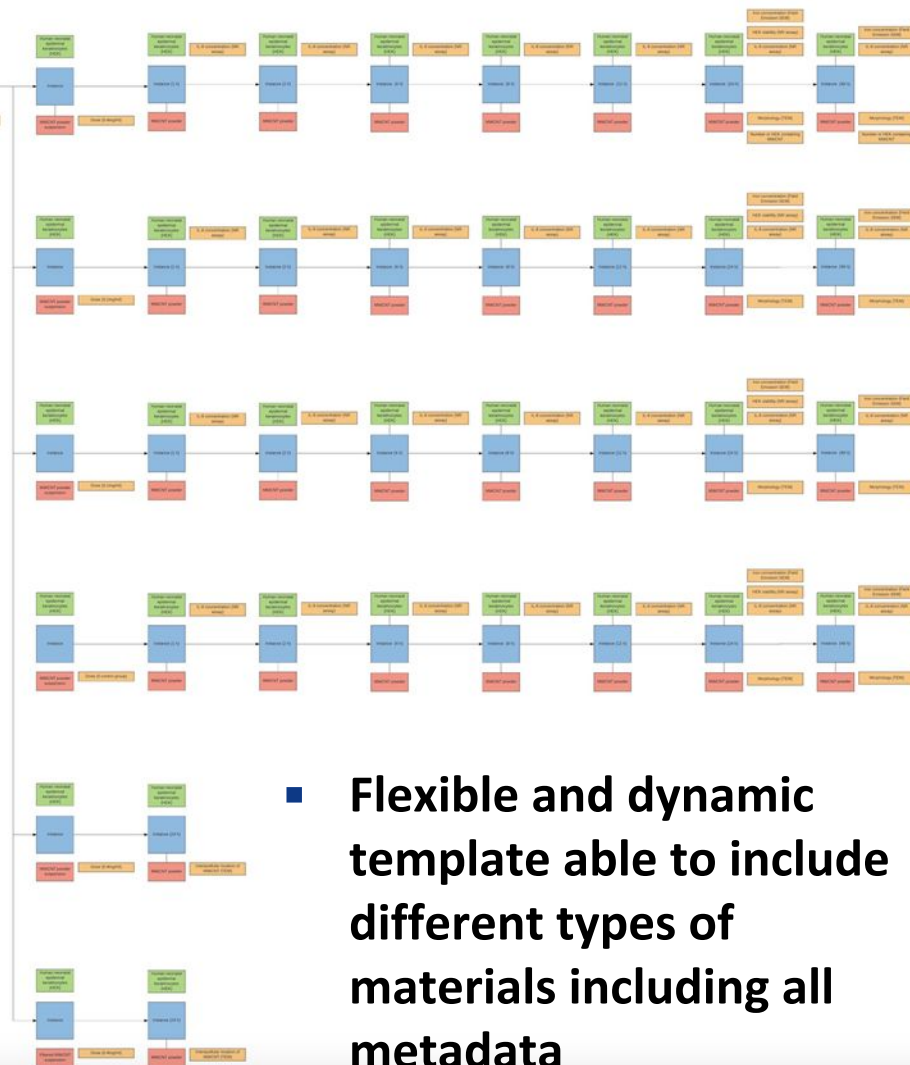
[Continue to next step](#)



# How to deal with different life cycle states?

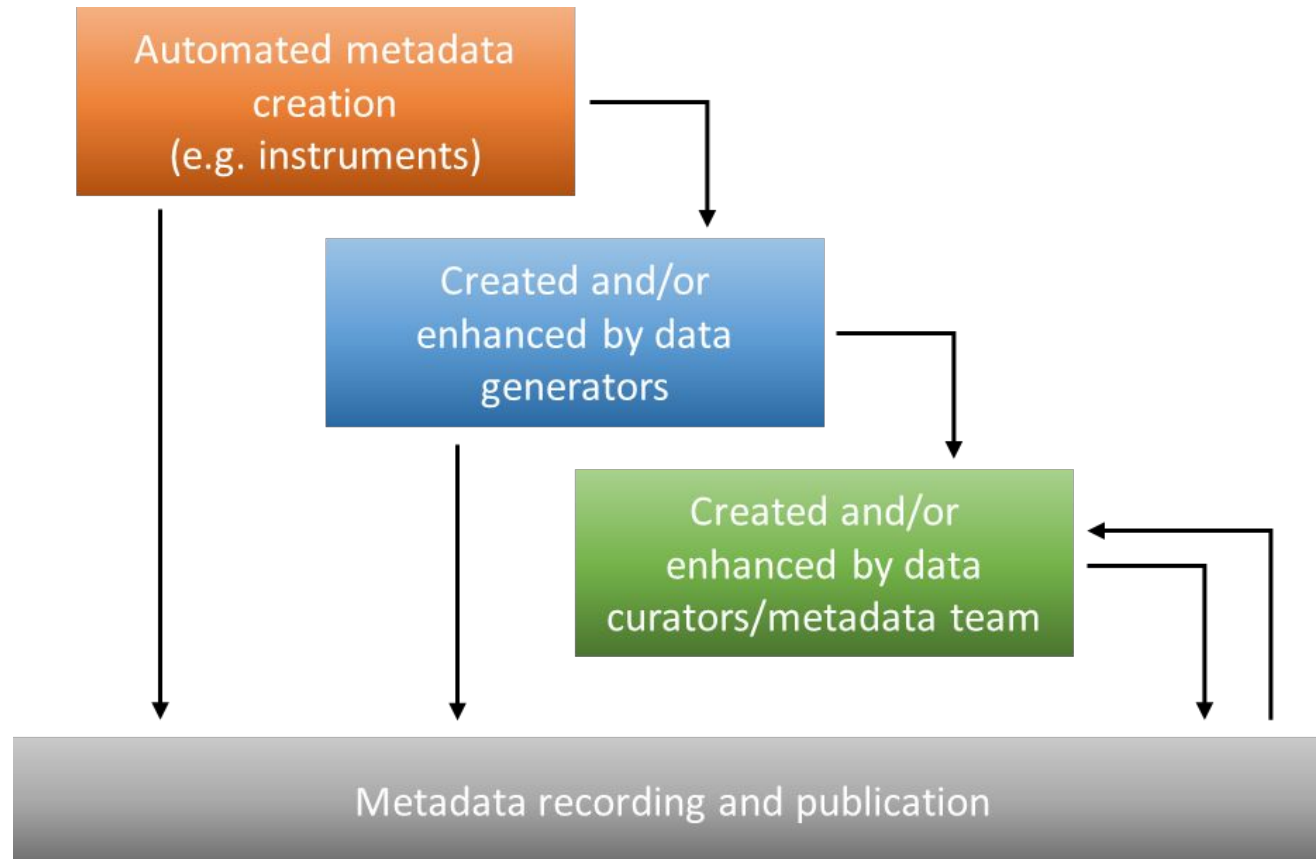


- The instance describes the lifecycle of nanomaterials



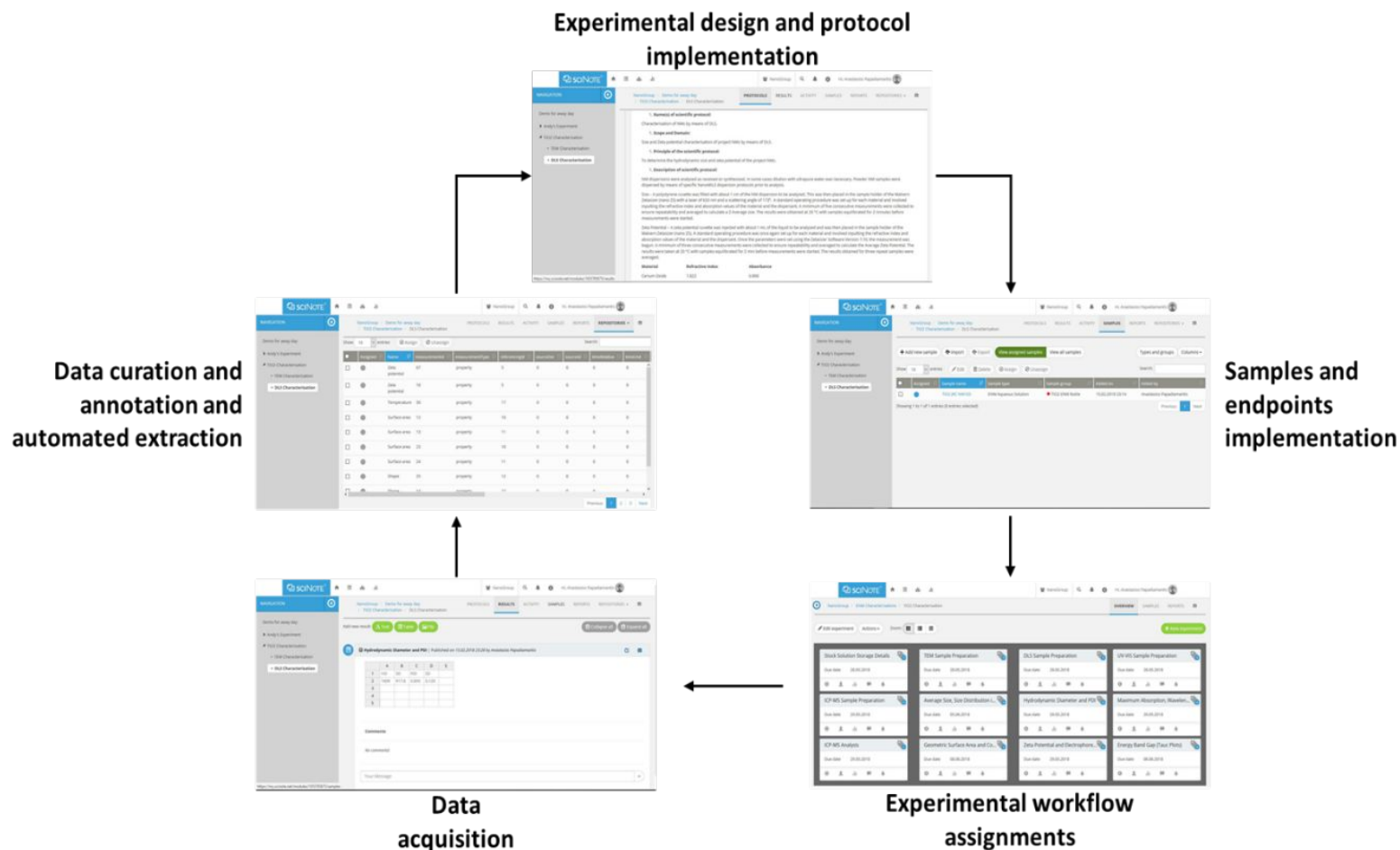
- Flexible and dynamic template able to include different types of materials including all metadata

# Curation standards and data stewardship



- It's not about the data, numbers mean nothing without context
- High quality metadata (methods, protocols, instruments) are needed to achieve maximum interoperability

# Integration into a full lab solution



- **Experimental workflow using Electronic Lab Notebooks**

# Annotation

# Ontology development and integration

## OpenRiskNet/NanoCommons ontology meeting

### Workshop, Hackathon (co-organized by OpenRiskNet)

13 – 14 Dec 2018 / Brussels, BE

### Activity details

The goal of this meeting is to get a picture of the ongoing ontology activities in the toxicology area, harmonize these efforts and the developed ontologies therein, and extend the existing toxicology ontology to support OpenRiskNet and NanoCommons tasks. Part of this will be the ontological annotation of OpenRiskNet Application Programming Interfaces (APIs) as used on their [cloud](#). Other goals include extension of the ontology with missing terms (if any), potentially write up guidance documents, and annotation of data sets (possible via OpenRiskNet data APIs). The detailed information and agenda are available below.

#### Topics:

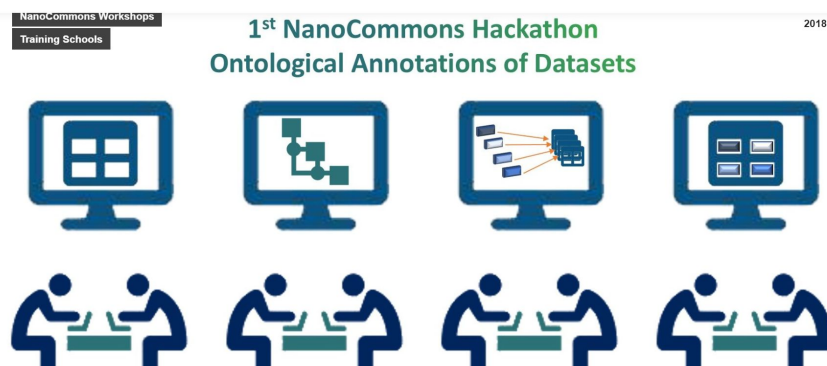
1. What ontologies are out there and can we combine them to a toxicology application ontology.
2. Data and software schema: How much ontology do we need to annotate complex services.
3. Ontology Hacking.

Available terms often not specific enough or misleading

→ More complex terms needed

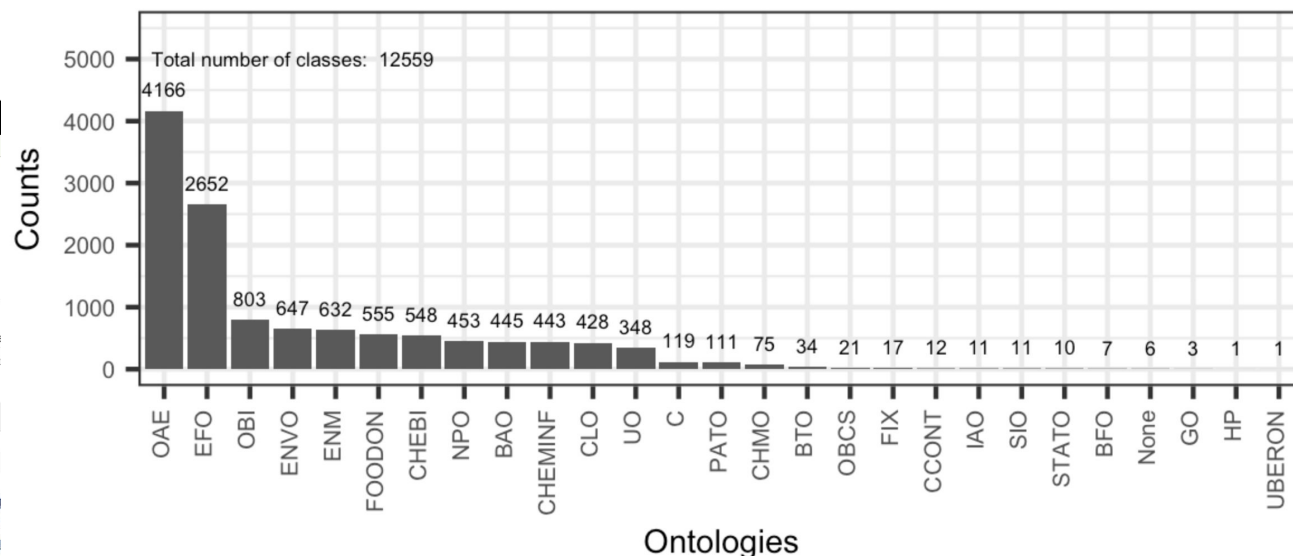
→ Better definitions

→ More training

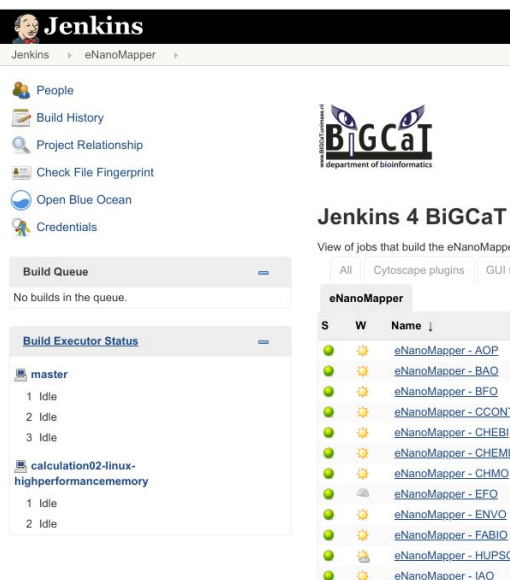


# Ontology development and integration

## eNanoMapper ontologies



Ontologies



**Jenkins 4 BiGCaT**  
View of jobs that build the eNanoMapper

**Build Queue**  
No builds in the queue.

**Build Executor Status**

S	W	Name
●	●	eNanoMapper - AOP
●	●	eNanoMapper - BAO
●	●	eNanoMapper - BFO
●	●	eNanoMapper - CCONT
●	●	eNanoMapper - CHEBI
●	●	eNanoMapper - CHEMI
●	●	eNanoMapper - CHMO
●	●	eNanoMapper - EFO
●	●	eNanoMapper - ENVO
●	●	eNanoMapper - FABIO
●	●	eNanoMapper - HUPSON
●	●	eNanoMapper - IAO

calculation02-linux-highperformancememory  
1 Idle  
2 Idle

## Releases after the management responsibility was transferred to NanoCommons:

5.0: 13 September 2018, 12,536 classes (update of CHEMINF)

5.0.1: 27 September 2018 (bug fixes)

5.0.2: 27 September 2018 (change in hosting)

6.0: 30 August 2019, 12,732 terms (addition of OECD Testing Guidelines)

# Additions needed for ACEnano

## Sample Analysis BET UoB test

### Measurement protocol

This protocol describes the measuring of the amount of physically adsorbed gas according to the Brunauer, Emmett and Teller (BET) method.

### Measurement

#### Endpoints

Endpoint: [http://www.bioassayontology.org/bao#BAO\\_0000179](http://www.bioassayontology.org/bao#BAO_0000179)

#### Technique

Technique: [http://purl.bioontology.org/ontology/npo#NPO\\_1405](http://purl.bioontology.org/ontology/npo#NPO_1405)

#### Type of raw data produced

Raw data: <http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C142663>

- BET Specific Surface Area using 5 isotherm data points at the adsorption branch of the isotherm within  $0.05 \leq p/p_0 \leq 0.2$
- C-constant
- $p/p_0$
- isotherm correlation coefficient

#### Measurement quality parameters

last adsorption isotherm data point taken at  $p/p_0$  – *common setting*: 0.2  
first isotherm data point taken at  $p/p_0$  – *common setting*: 0.01- 0.05

#### Phase in which the measurement is performed

Powder

# **Links to other NanoCommons services and how to find relevant Transnational Access offerings**



# Tools for data search and retrieval: data APIs

Response Content Type

Parameters

Parameter	Value	Description	Parameter Type	Data Type
Authorization	<input type="text"/>	Authorization token	header	string
id	<input type="text" value="8aaf68b299f14fa28721131715e2c3af"/>		path	string
dataEntries	<input type="text" value="true"/>		query	boolean
rowStart	<input type="text"/>		query	integer
rowMax	<input type="text"/>		query	integer
colStart	<input type="text"/>		query	integer
colMax	<input type="text"/>		query	integer
stratify	<input type="text"/>		query	boolean
seed	<input type="text"/>		query	boolean
folds	<input type="text"/>		query	integer
target_feature	<input type="text"/>		query	boolean

Response Messages

HTTP Status Code	Reason
------------------	--------

```
import http.client as http_client
import logging
import json
import pandas as pd
import numpy as np
from jaxpotpy import Jaxpot
```

```
user = "Hackathon"
```

```
pw = getpass.getpass("Login password for user '{}': ".format(user))
```

```
url = "https://ssl.biomax.de/nanocommons/bioxm/rest/api"
```

```
proxies = {
    #'https': 'server:8080'
}
```

## OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE

```
on...")
```

```
=
```

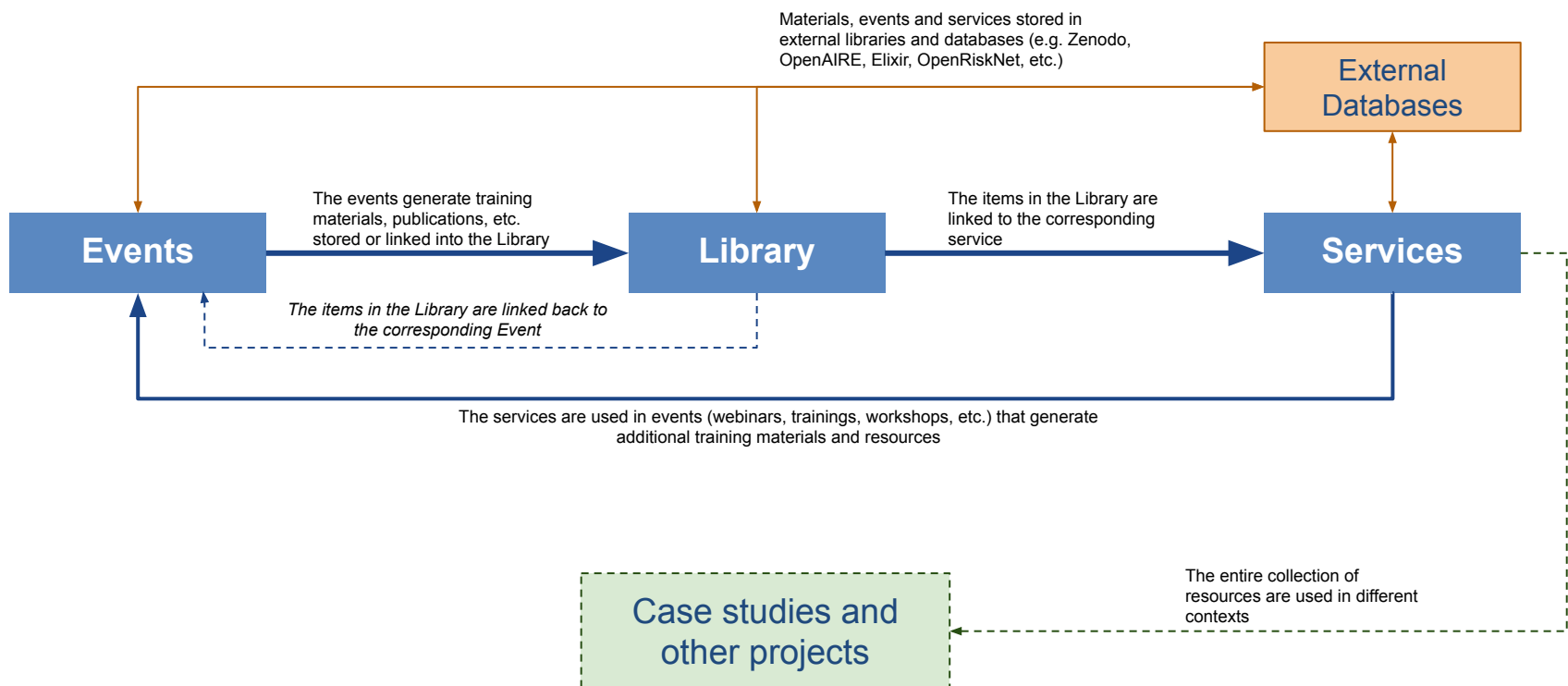
```
requests.get(url
```

```
Simple?name={}&password={}".format(user, pw),
es=proxies)
```

```
+
```

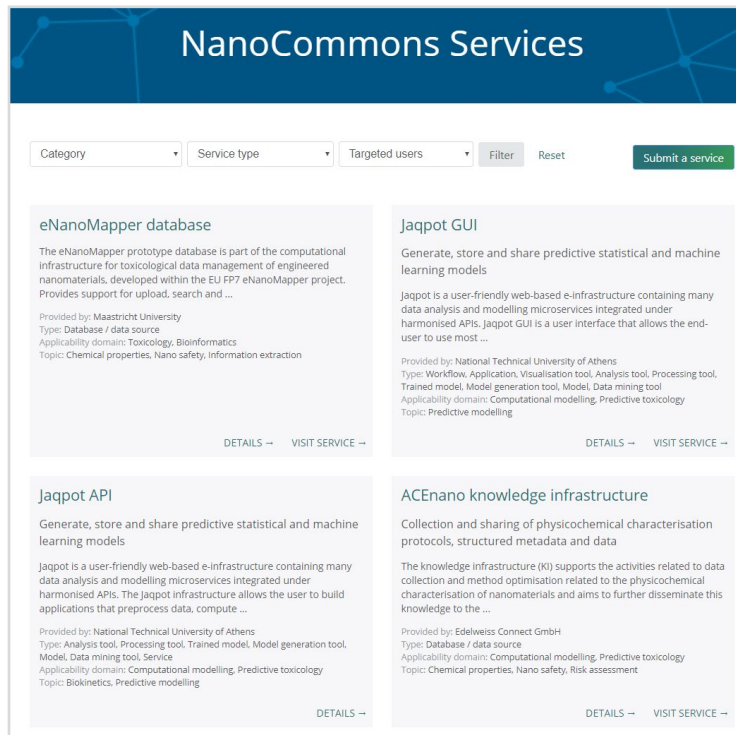
# Service descriptions and discover service

Concept implemented in OpenRiskNet e-infrastructure  
and adapted for NanoCommons infrastructure



# Service descriptions and discover service

- The catalogue provides a detailed description of the services, and provides direct links to the service environment, their APIs and to all related support resources.
- The catalogue supports the users in filtering the information on services offered offerings and the corresponding tools based on predefined descriptors.
- List of relevant Events (organised or attended by NanoCommons members) and resources gathered in the Library section (e.g. training materials, publications, etc.)



The screenshot shows the 'NanoCommons Services' web interface. At the top, there's a blue header with the title. Below it, a search bar contains filters for 'Category', 'Service type', and 'Targeted users', along with 'Filter', 'Reset', and 'Submit a service' buttons. The main content area displays four service cards:

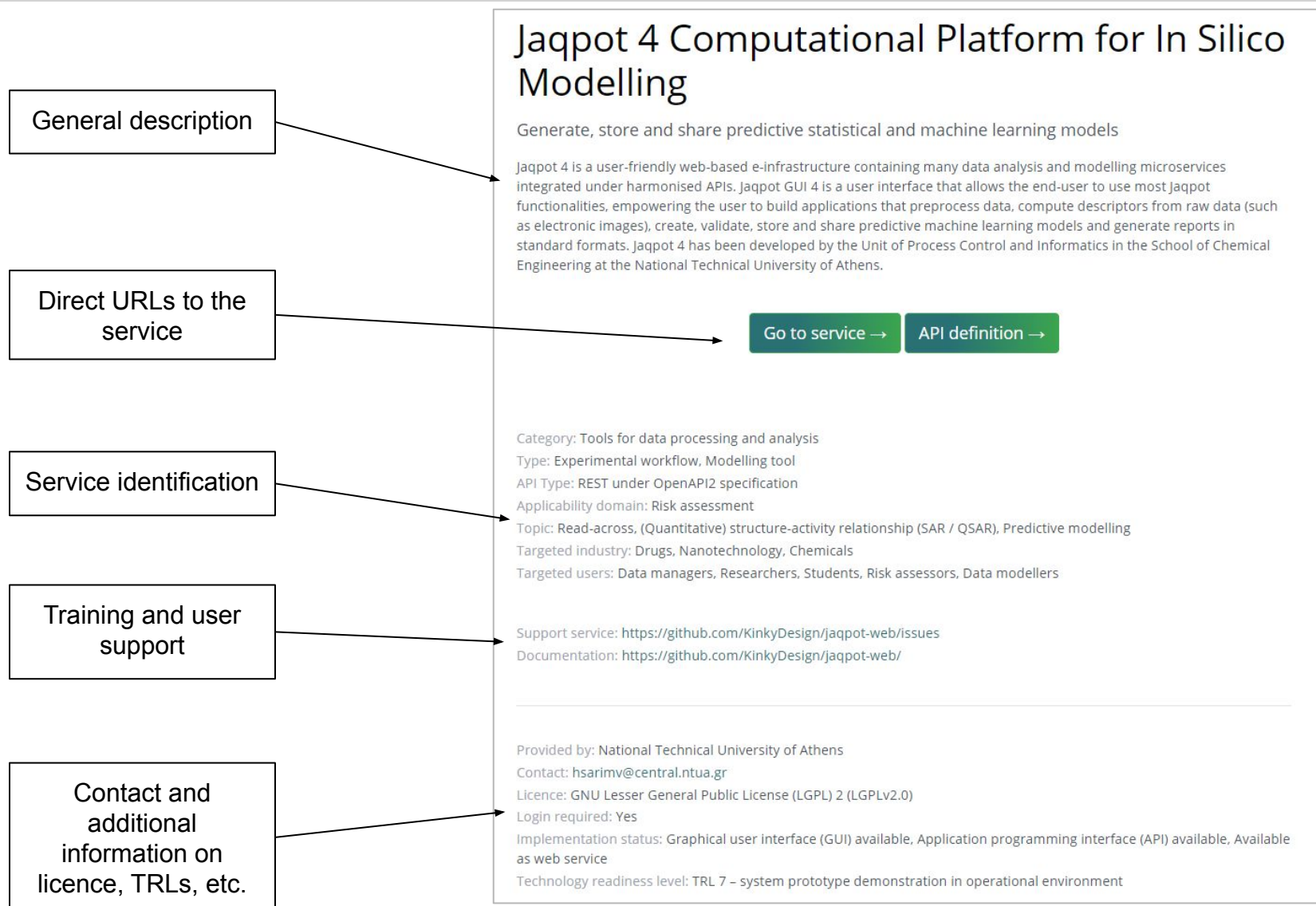
- eNanoMapper database**: A computational infrastructure for toxicological data management of engineered nanomaterials. Provided by Maastricht University. Type: Database / data source. Applicability domain: Toxicology, Bioinformatics. Topic: Chemical properties, Nano safety, Information extraction.
- Jaqpote GUI**: Generate, store and share predictive statistical and machine learning models. Jaqpote is a user-friendly web-based e-infrastructure containing many data analysis and modelling microservices integrated under harmonised APIs. Jaqpote GUI is a user interface that allows the end-user to use most ... Provided by: National Technical University of Athens. Type: Workflow, Application, Visualisation tool, Analysis tool, Processing tool, Trained model, Model generation tool, Model, Data mining tool. Applicability domain: Computational modelling, Predictive toxicology. Topic: Predictive modelling.
- Jaqpote API**: Generate, store and share predictive statistical and machine learning models. Jaqpote is a user-friendly web-based e-infrastructure containing many data analysis and modelling microservices integrated under harmonised APIs. The Jaqpote infrastructure allows the user to build applications that preprocess data, compute ... Provided by: National Technical University of Athens. Type: Analysis tool, Processing tool, Trained model, Model generation tool, Model, Data mining tool, Service. Applicability domain: Computational modelling, Predictive toxicology. Topic: Biokinetics, Predictive modelling.
- ACEnano knowledge infrastructure**: Collection and sharing of physicochemical characterisation protocols, structured metadata and data. The knowledge infrastructure (KI) supports the activities related to data collection and method optimisation related to the physicochemical characterisation of nanomaterials and aims to further disseminate this knowledge to the ... Provided by: Edelweiss Connect GmbH. Type: Database / data source. Applicability domain: Computational modelling, Predictive toxicology. Topic: Chemical properties, Nano safety, Risk assessment.

Each card has 'DETAILS' and 'VISIT SERVICE' links at the bottom.

- **Web:** <https://infrastructure.nanocommons.eu/>

Service identification
Name
URL
API URL
API Type
Provider name
Provider contact
Provider organisation
Service description
Tagline
Description
Category
Service type
Implementation status
Technology readiness level
Applicability domain
Topic
Targeted industry
Targeted users
Licence
Training and user support
User support service
User support contact
Documentation center
References

# Service descriptions and discover service



# Conclusion

# Call to action

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- Get involved!
- NanoCommons is looking to promote scientific data collaboration at a global scale
- We are looking to expand our Community and promote FAIR and Open data
- Contact us:
  - [Thomas.Exner@edelweissconnect.com](mailto:Thomas.Exner@edelweissconnect.com)
  - [A.Papadiamantis@bham.ac.uk](mailto:A.Papadiamantis@bham.ac.uk)
  - [I.Lynch@bham.ac.uk](mailto:I.Lynch@bham.ac.uk)
- Visit [www.nanocommons.eu](http://www.nanocommons.eu) and subscribe to receive our Transnational Access calls to take advantage of our free services
- Promote FAIR data!

# Conclusions

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*“Open Data is going to help launch more startups. It’s going to help launch more businesses ... It’s going to help more entrepreneurs come up with products and services that we haven’t even imagined yet”.*

**Former US President Barack Obama, May, 2013  
Middle Class Jobs and Opportunity Tour**

*Thank you*



*for your attention!*

**NanoCommons**

Nano-Knowledge Community

Dieter Maier  
BioMax Informatics AG

Iseult Lynch, Tassos Papadiamantis  
University of Birmingham

Joh Dokler, Lucian Farcas,  
Maja Brajnik  
Edelweiss Connect GmbH

Egon Willighagen  
Maastricht University

***NanoSafety Cluster week  
Copenhagen, 9 October 2019***



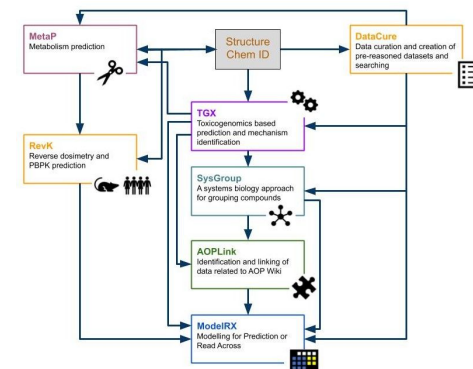
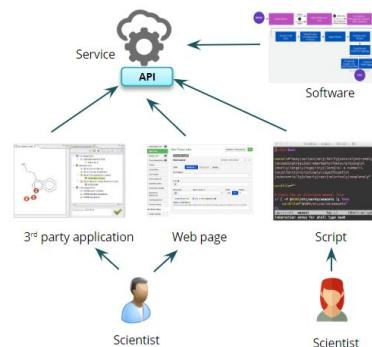
# OpenRiskNet, an open e-infrastructure to support data sharing, knowledge integration and *in silico* analysis and modelling in predictive toxicology and risk assessment (Grant number: 731075)

OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE



**H2020-EINFRA** Call  
**2016-2019** 3 years project  
**3 mil** Total funding  
**11** Partner Organisations  
**14** Associated Partners  
**7** Case studies



E-infrastructure providing resources and services to a variety of communities requiring risk assessment, including **chemicals, cosmetic ingredients, therapeutic agents and nanomaterials**:

- **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**.



P1 Edelweiss Connect GmbH, Switzerland (EwC)  
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)  
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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)

## Final Workshop

Creating powerful workflows combining data and software services demonstrated on risk assessment case studies

**23 - 24 October 2019**  
**Amsterdam, Netherlands**

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