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

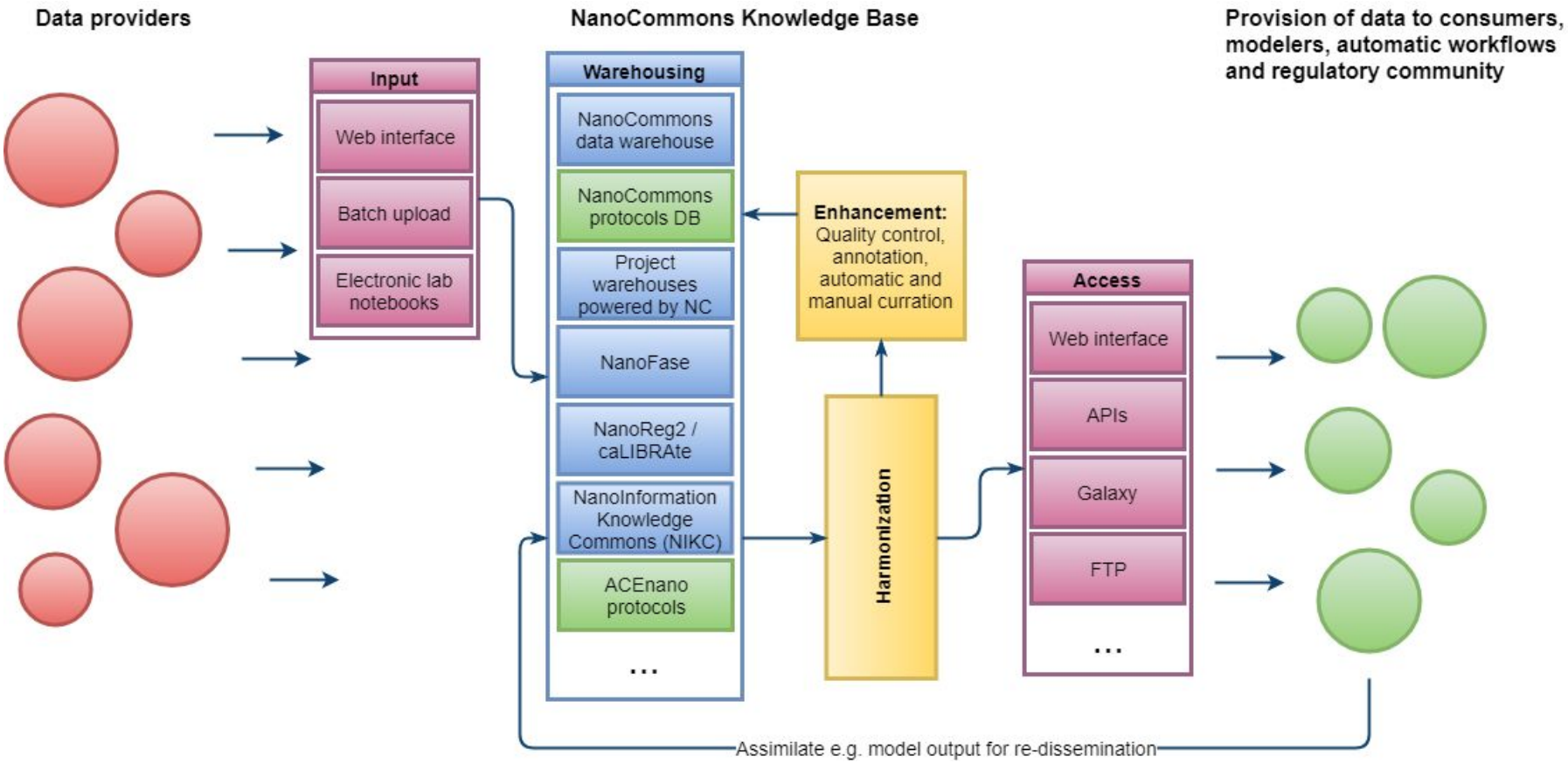
built to support the research communities, industrial users and regulators in the area of nanomaterials safety assessment

Thomas Exner - Edelweiss Connect

NanoSafety Cluster week
Copenhagen, 9 October 2019

Data Driven Innovation – Added Value

Scope of the data management tasks



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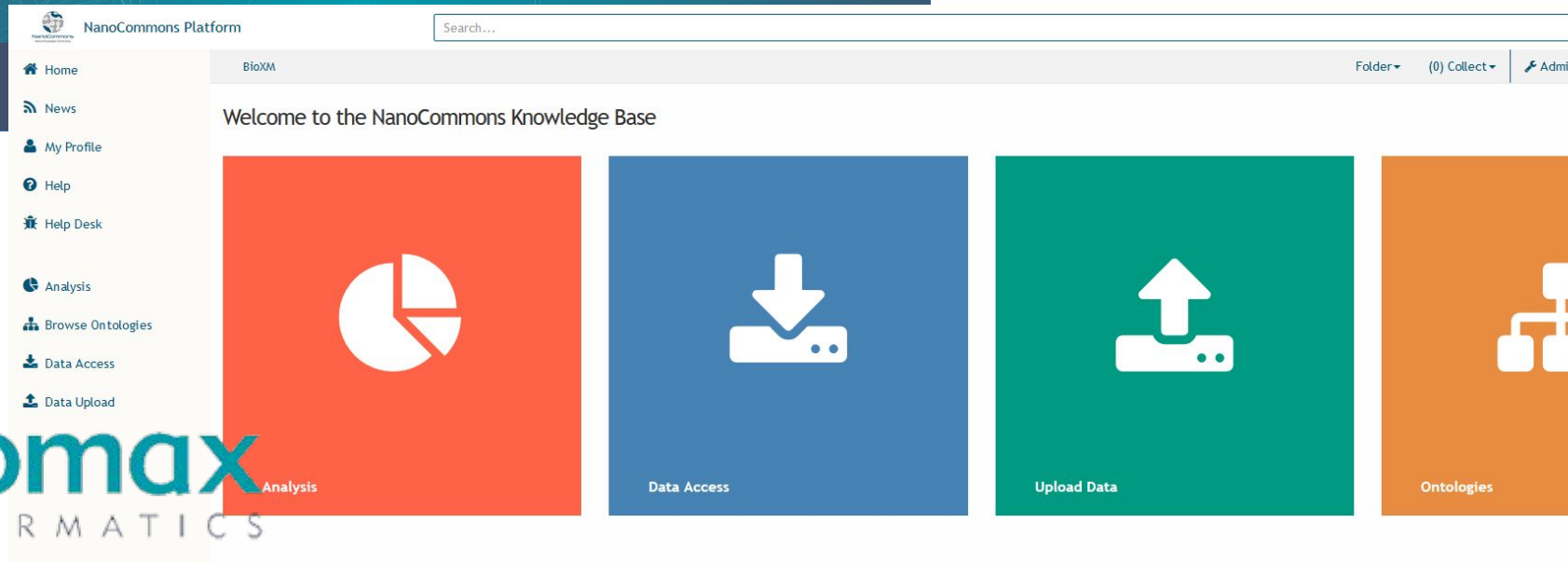
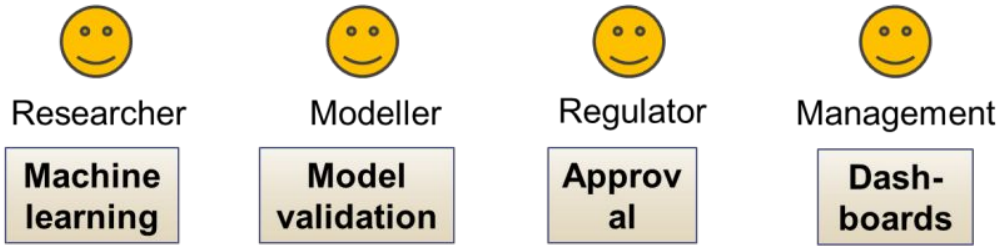
Data management and sharing

NanoCommons Knowledge Infrastructure



Biomax INFORMATICS

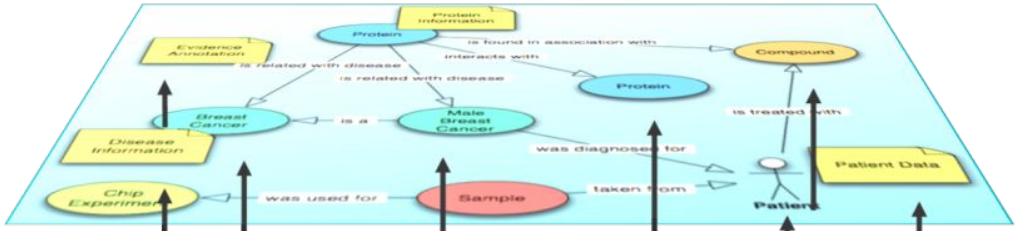
Why is it more than data warehousing?



UI ⇧ **API**

Query, analyse based on Semantic Model

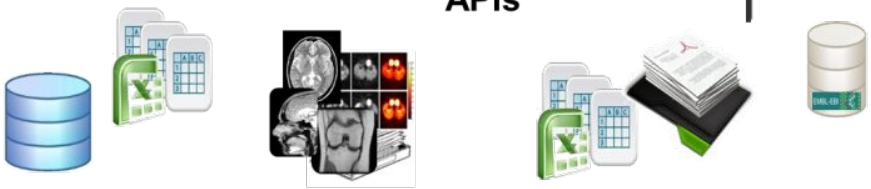
Semantic Model



Semantically integrate any kind of data

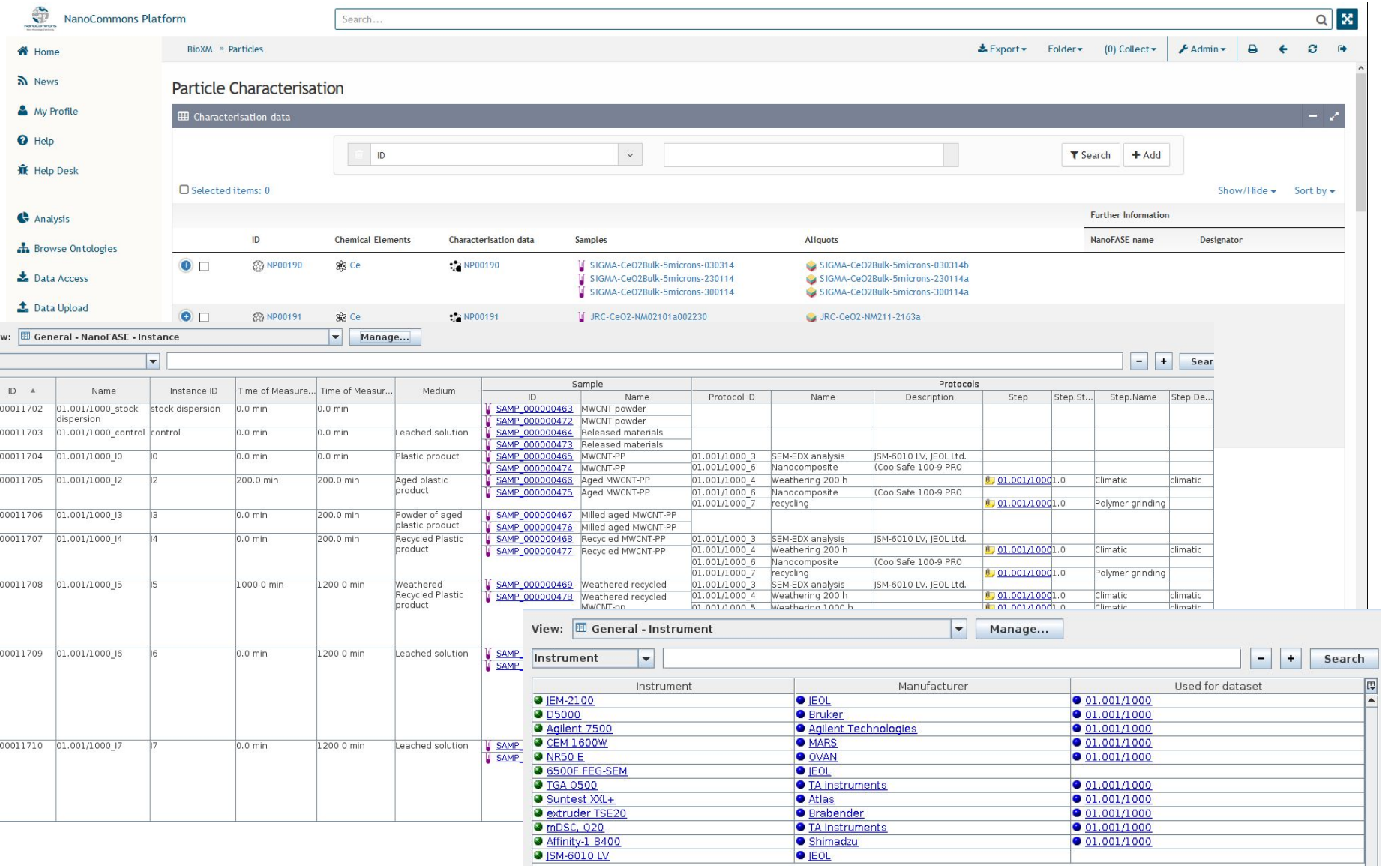
APIs

Original DBs



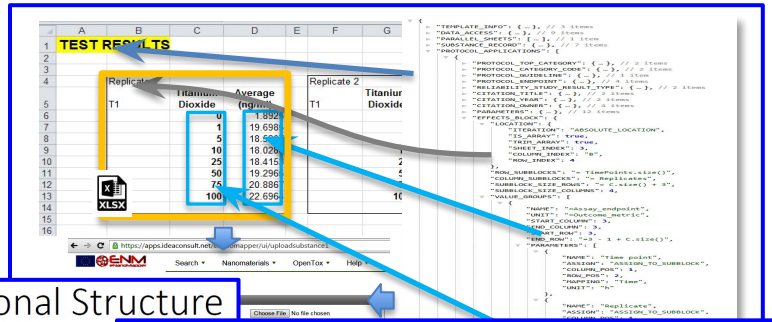
NanoMILE/NanoFASE/NanoReg/eNanoMapper

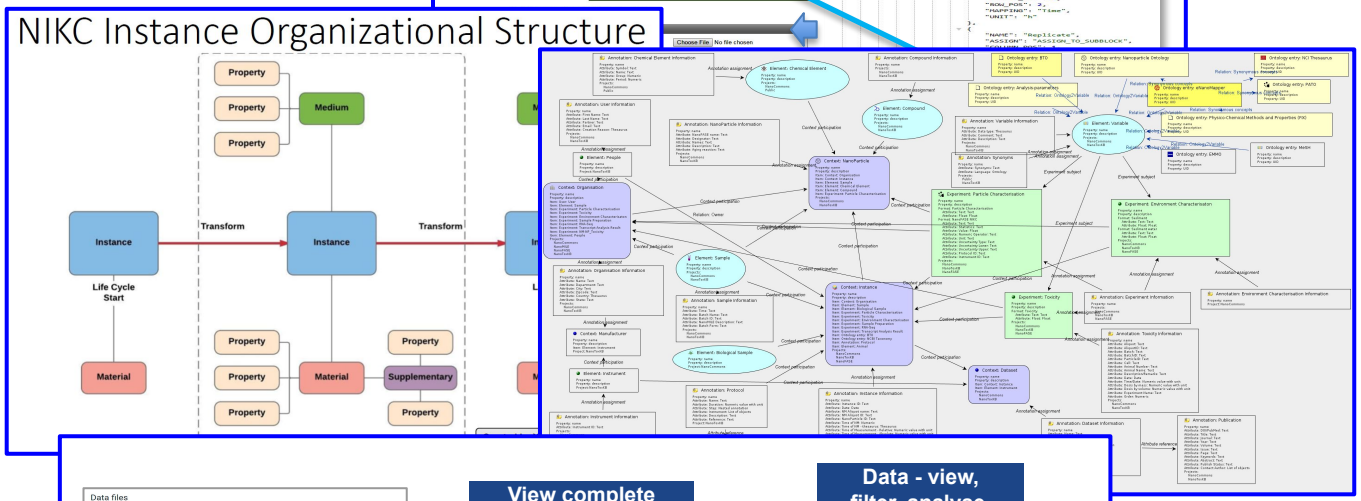
NanoCommons data warehouse

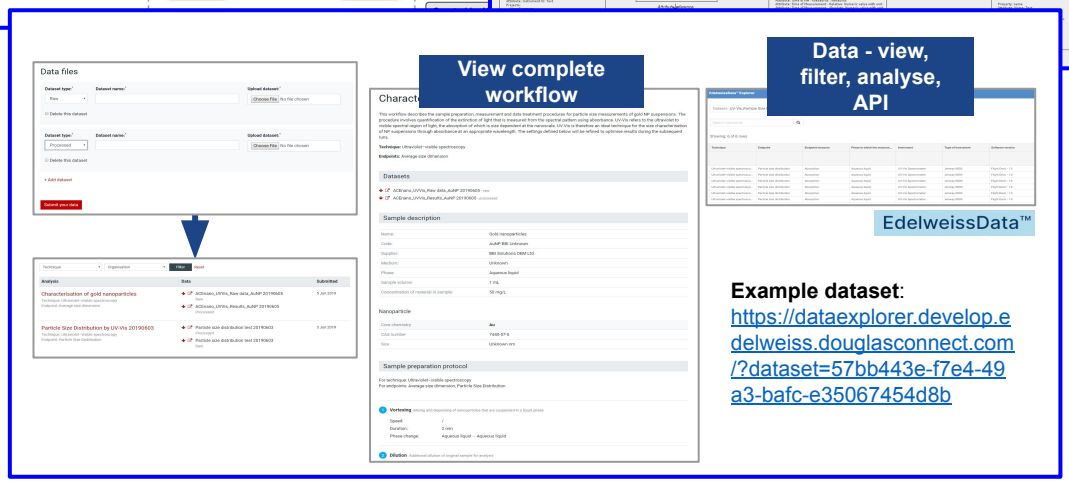


Data warehousing: external data sources

- eNanoMapper
- NIKC and NanoFase
- ACEnano







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Data quality

Data management and data lifecycle

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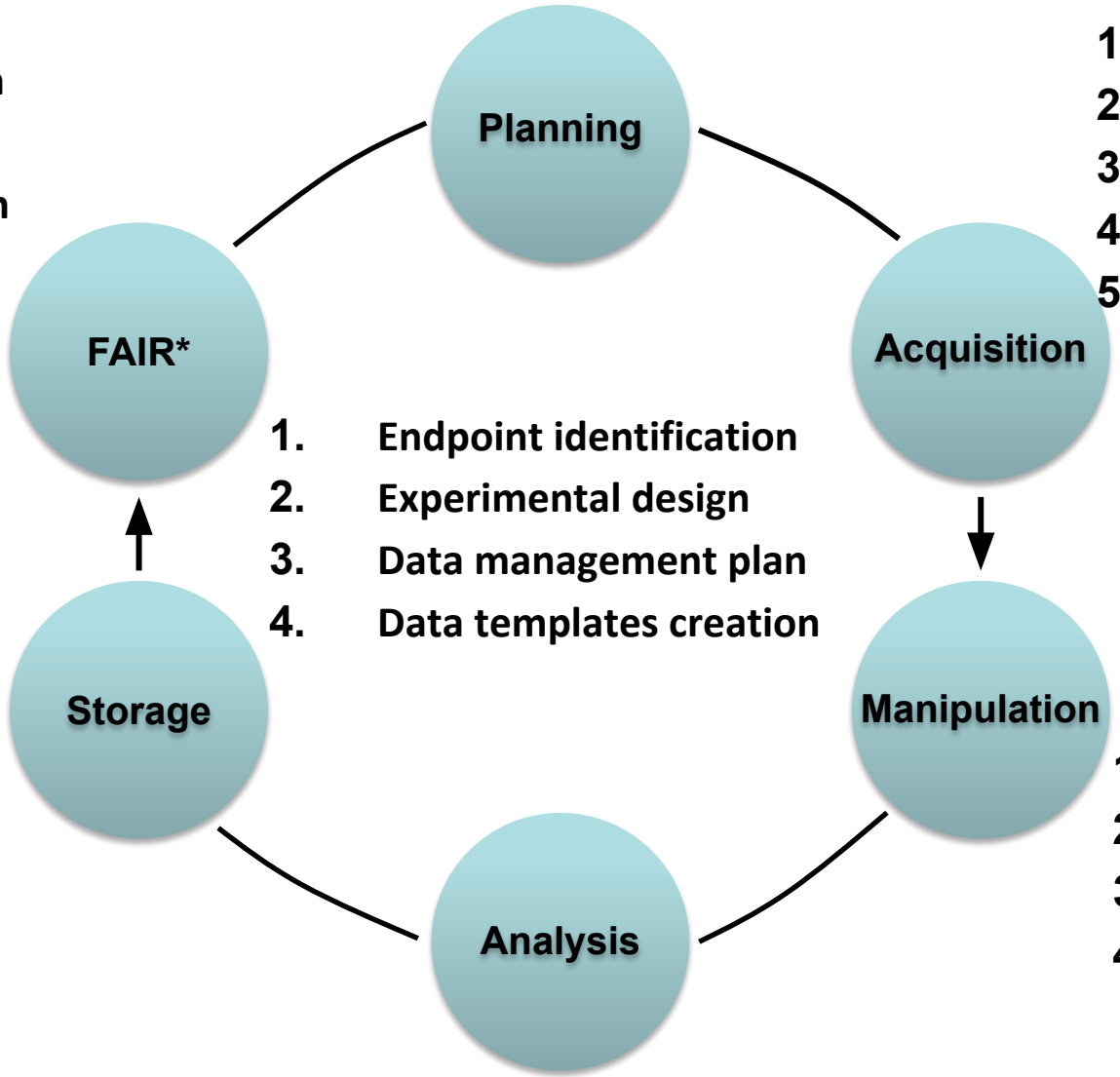

. Data acquisition
. Data curation
. Data digitisation

etation
QSARs/Omics
tputs

1. Endpoint identification
2. Experimental design
3. Data management plan
4. Data templates creation

1. Backup and stor
2. Assign DOI
3. Create metadata
4. Prepare docume
5. Online access

1. Data Quality Co
2. Data cleansing
3. Storage
4. Tools implemen

*Findable, Accessible, Interoperable, Reusable

Data management, data lifecycle & metadata

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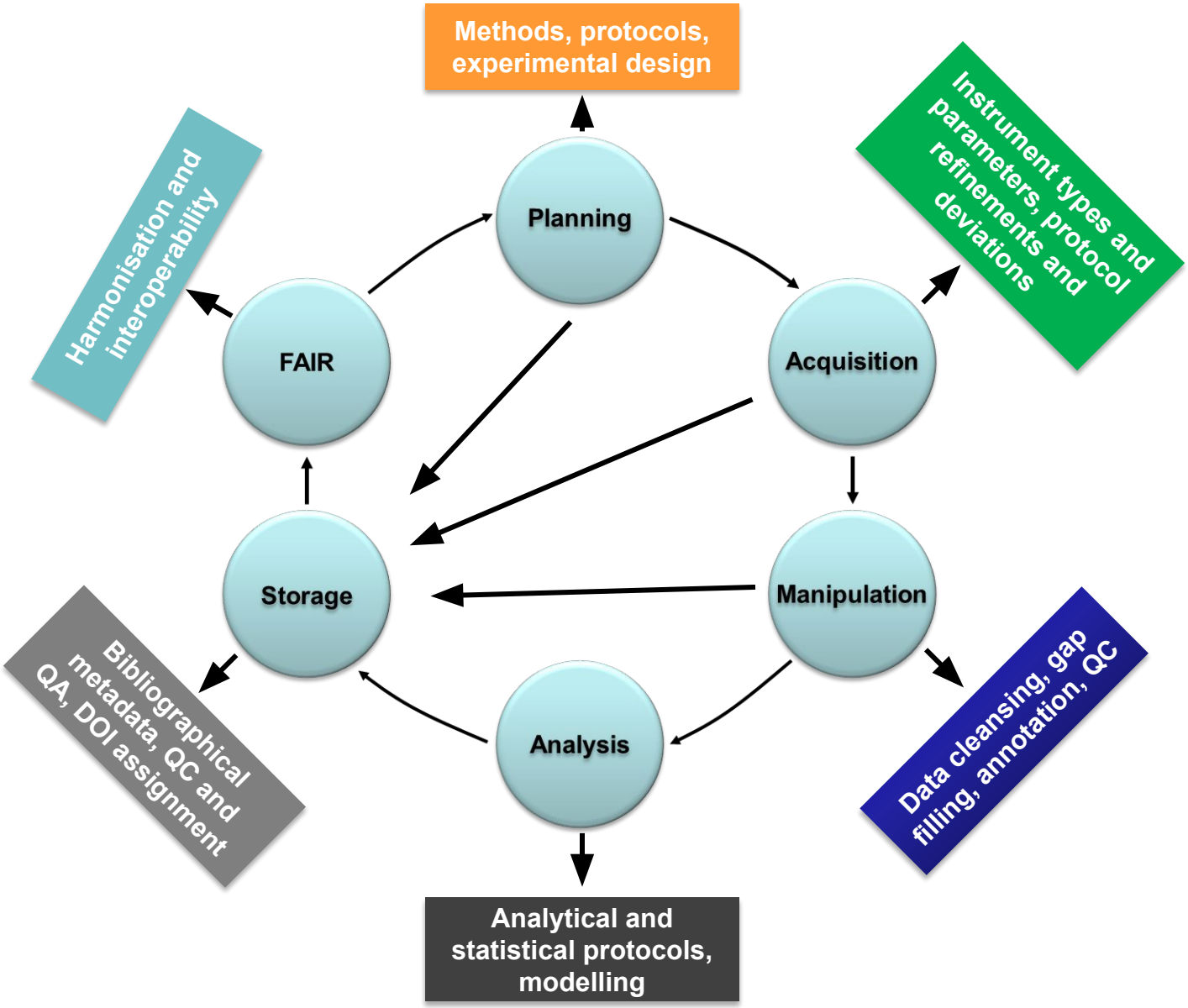

Can we harmonize data capturing?

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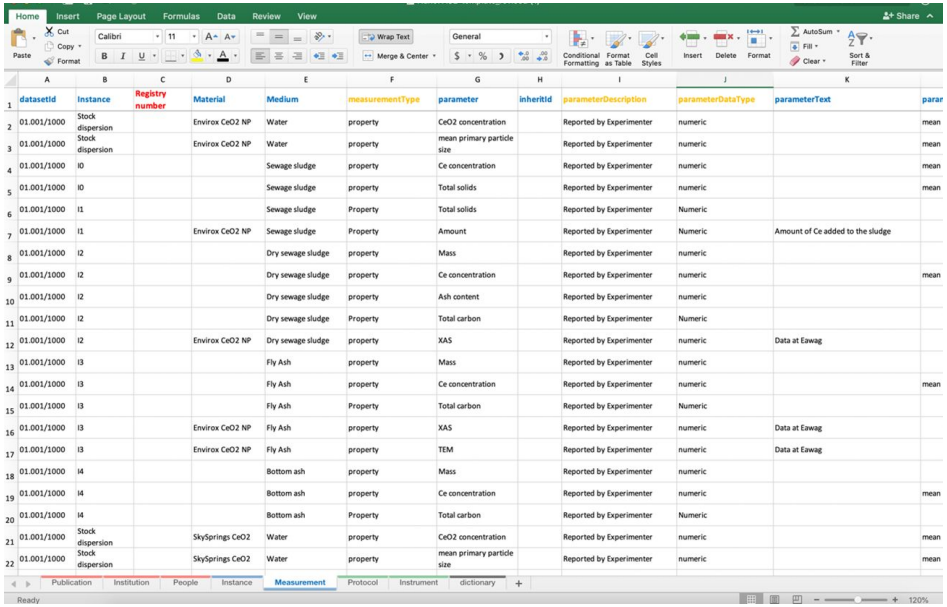
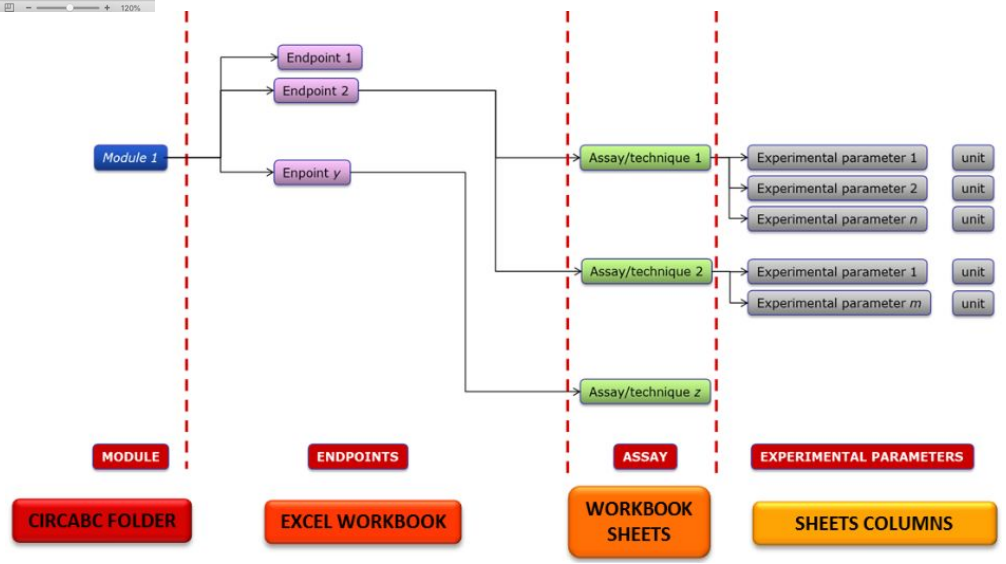


	A	B	C	D	E	F	G	H	I	J	K	
1	datasetId	Instance	Registry number	Material	Medium	measurementType	parameter	inheritId	parameterDescription	parameterDataType	parameterText	parar
2	01.001/1000	Stock dispersion		Envirox CeO2 NP	Water	property	CeO2 concentration		Reported by Experimenter	numeric		mean
3	01.001/1000	Stock dispersion		Envirox CeO2 NP	Water	property	mean primary particle size		Reported by Experimenter	numeric		mean
4	01.001/1000	I0			Sewage sludge	property	Ce concentration		Reported by Experimenter	numeric		mean
5	01.001/1000	I0			Sewage sludge	property	Total solids		Reported by Experimenter	numeric		mean
6	01.001/1000	I1			Sewage sludge	Property	Total solids		Reported by Experimenter	Numeric		
7	01.001/1000	I1		Envirox CeO2 NP	Sewage sludge	Property	Amount		Reported by Experimenter	Numeric	Amount of Ce added to the sludge	
8	01.001/1000	I2			Dry sewage sludge	property	Mass		Reported by Experimenter	numeric		
9	01.001/1000	I2			Dry sewage sludge	property	Ce concentration		Reported by Experimenter	numeric		mean
10	01.001/1000	I2			Dry sewage sludge	property	Ash content		Reported by Experimenter	numeric		
11	01.001/1000	I2			Dry sewage sludge	Property	Total carbon		Reported by Experimenter	Numeric		
12	01.001/1000	I2		Envirox CeO2 NP	Dry sewage sludge	property	XAS		Reported by Experimenter	numeric	Data at Eawag	
13	01.001/1000	I3			Fly Ash	property	Mass		Reported by Experimenter	numeric		
14	01.001/1000	I3			Fly Ash	property	Ce concentration		Reported by Experimenter	numeric		mean
15	01.001/1000	I3			Fly Ash	Property	Total carbon		Reported by Experimenter	Numeric		
16	01.001/1000	I3		Envirox CeO2 NP	Fly Ash	property	XAS		Reported by Experimenter	numeric	Data at Eawag	
17	01.001/1000	I3		Envirox CeO2 NP	Fly Ash	property	TEM		Reported by Experimenter	numeric	Data at Eawag	
18	01.001/1000	I4			Bottom ash	property	Mass		Reported by Experimenter	numeric		
19	01.001/1000	I4			Bottom ash	property	Ce concentration		Reported by Experimenter	numeric		mean
20	01.001/1000	I4			Bottom ash	Property	Total carbon		Reported by Experimenter	Numeric		
21	01.001/1000	Stock dispersion		SkySprings CeO2	Water	property	CeO2 concentration		Reported by Experimenter	numeric		mean
22	01.001/1000	Stock dispersion		SkySprings CeO2	Water	property	mean primary particle size		Reported by Experimenter	numeric		mean

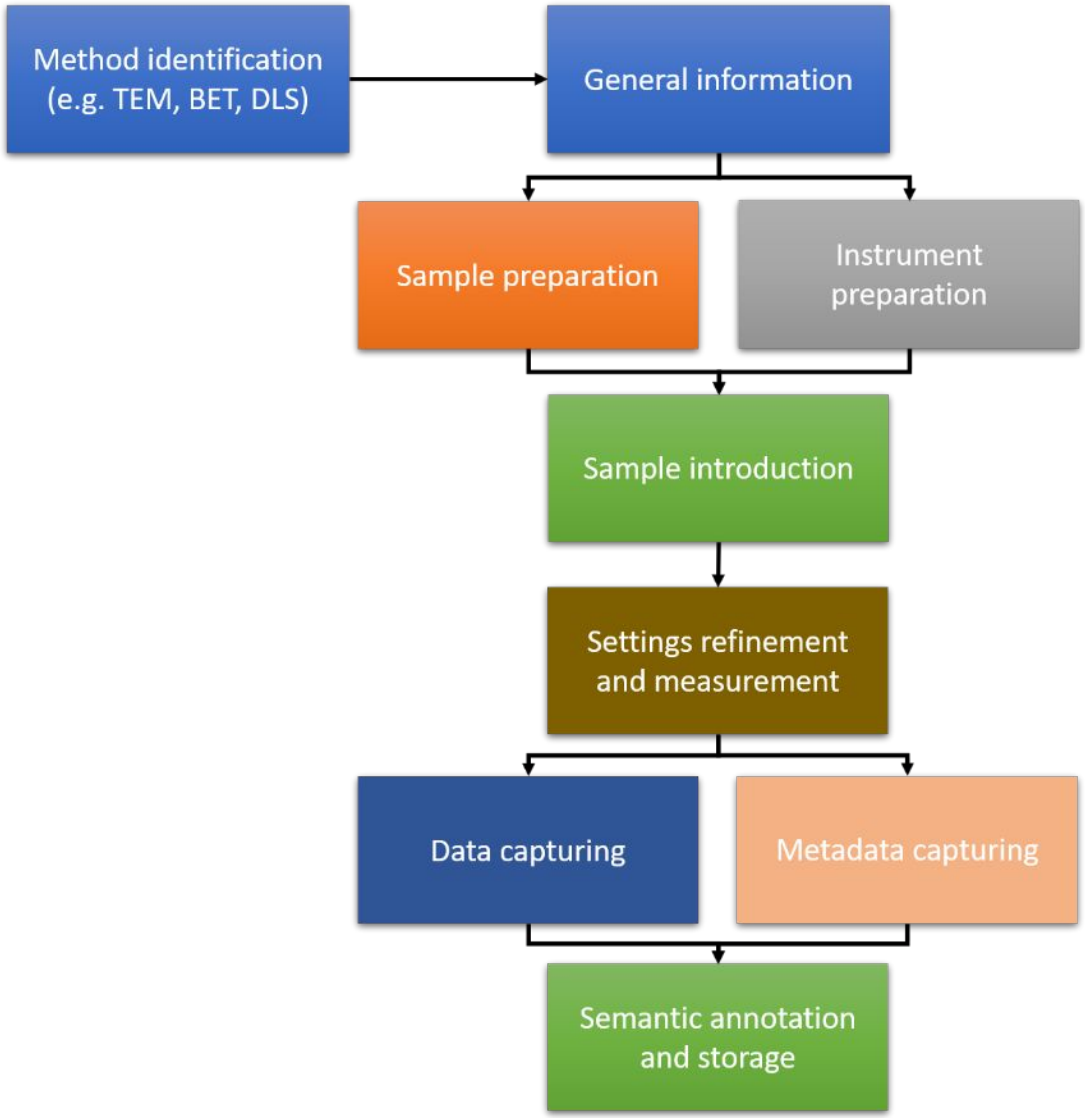
NIKC

NanoREG templates



- **Evaluation of data capturing templates.**

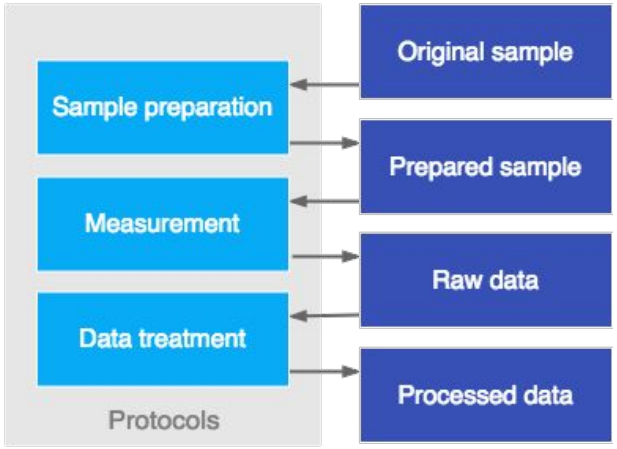
Protocols capturing workflow



Appoach to protocols and data

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

Protocols: measurement

Part 2: Equipment

Equipment

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

Name:* **Model:** **Instrument typ**

Common instrument makes and models.

Software: **Software version:**

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

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	delete
Setting	Value	Unit	delete
Setting	Value	Unit	delete

Possible datasets

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

Axe:* **Units:** Delete

+ Add another axe

Measurement quality parameters

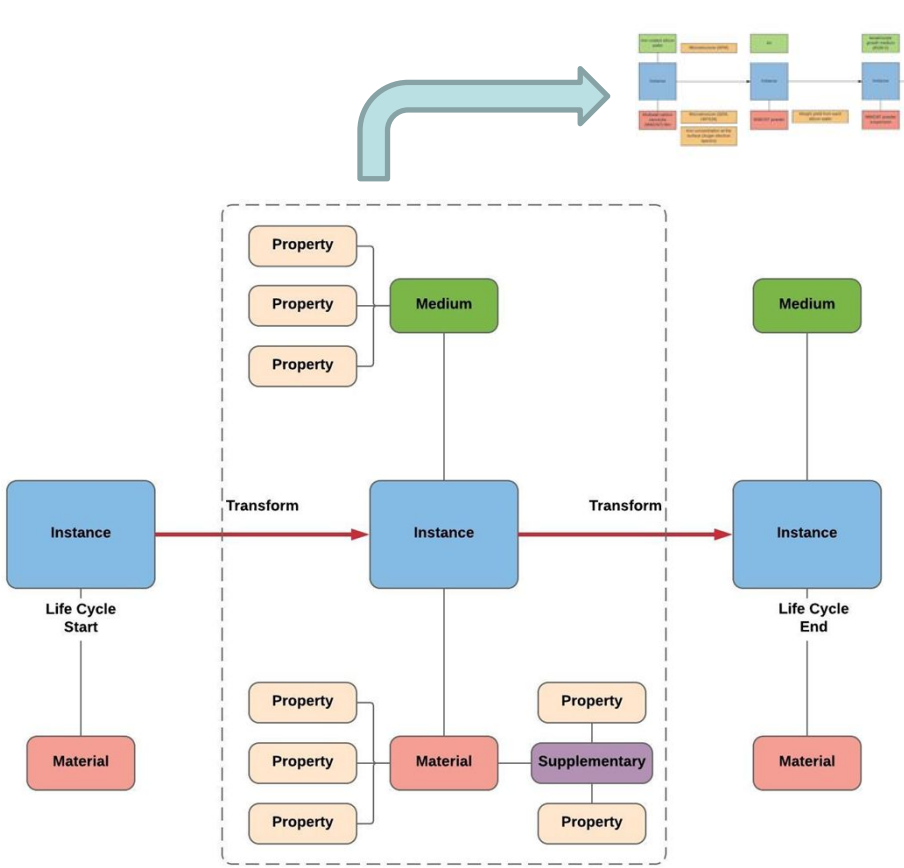
State parameters that are measured by the instrument that give an indication of the accuracy or also their units if applicable.

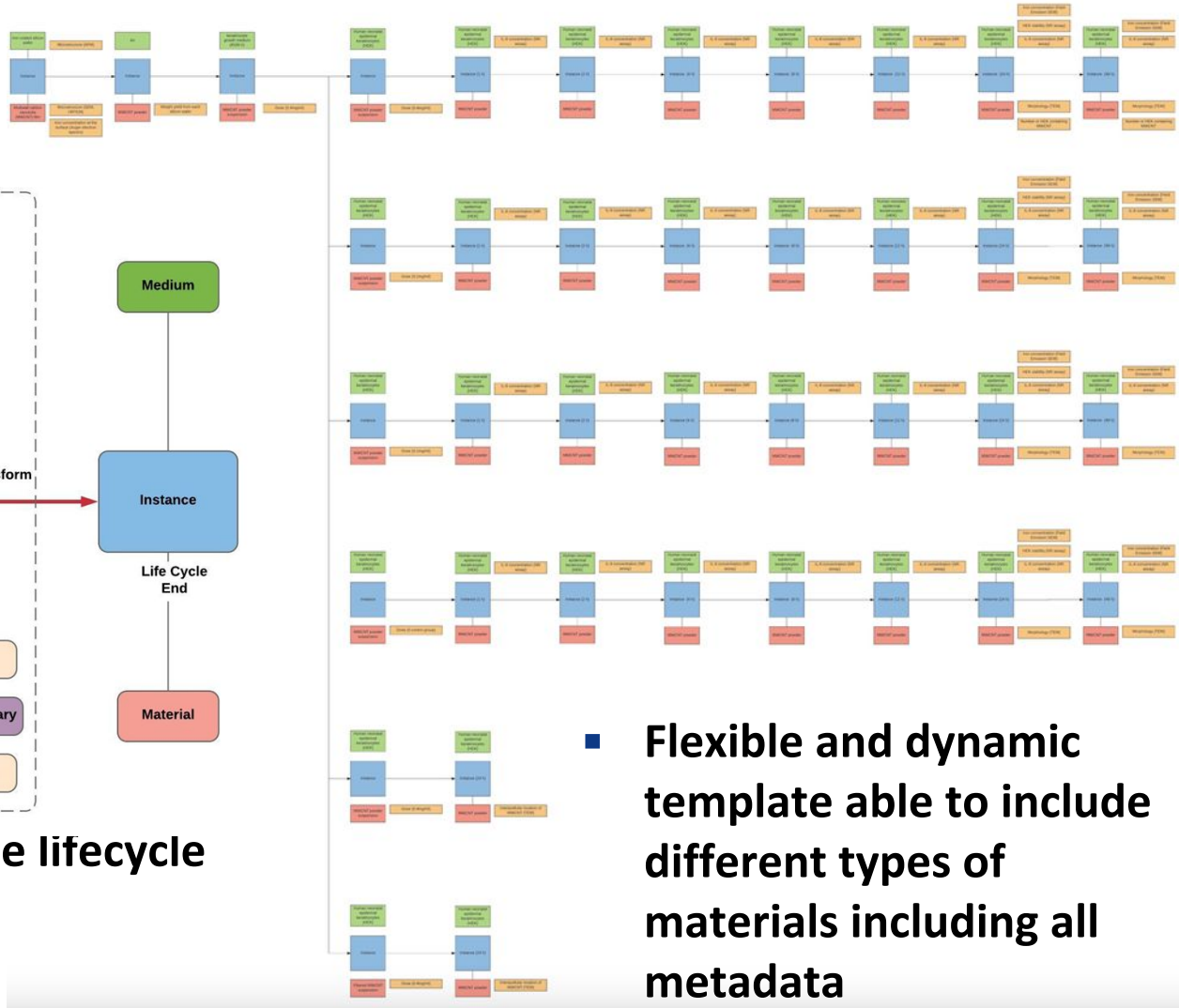
Parameter:* **Common setting:** **Units:**

+ Add another quality parameter

Continue to next step

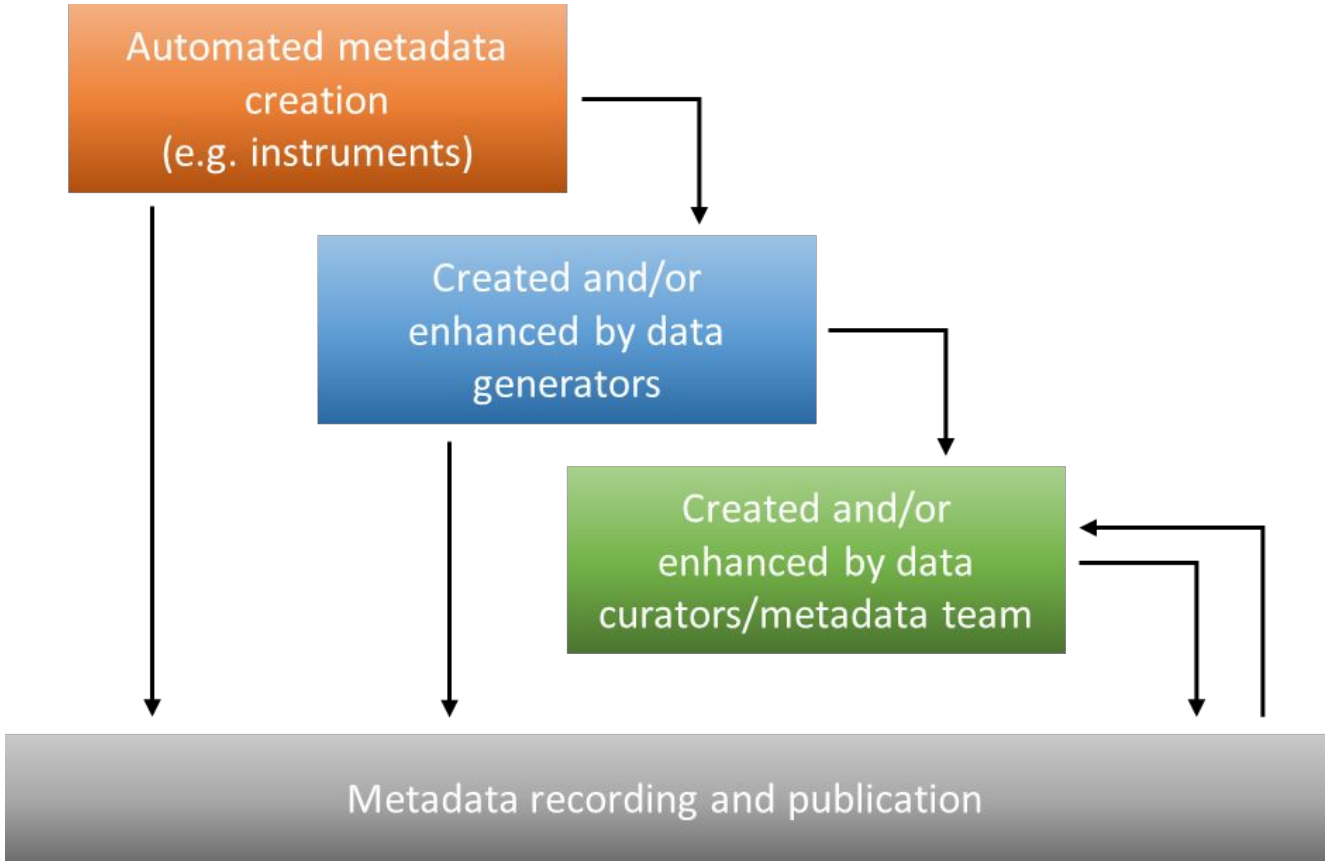
How to deal with different life cycle states?





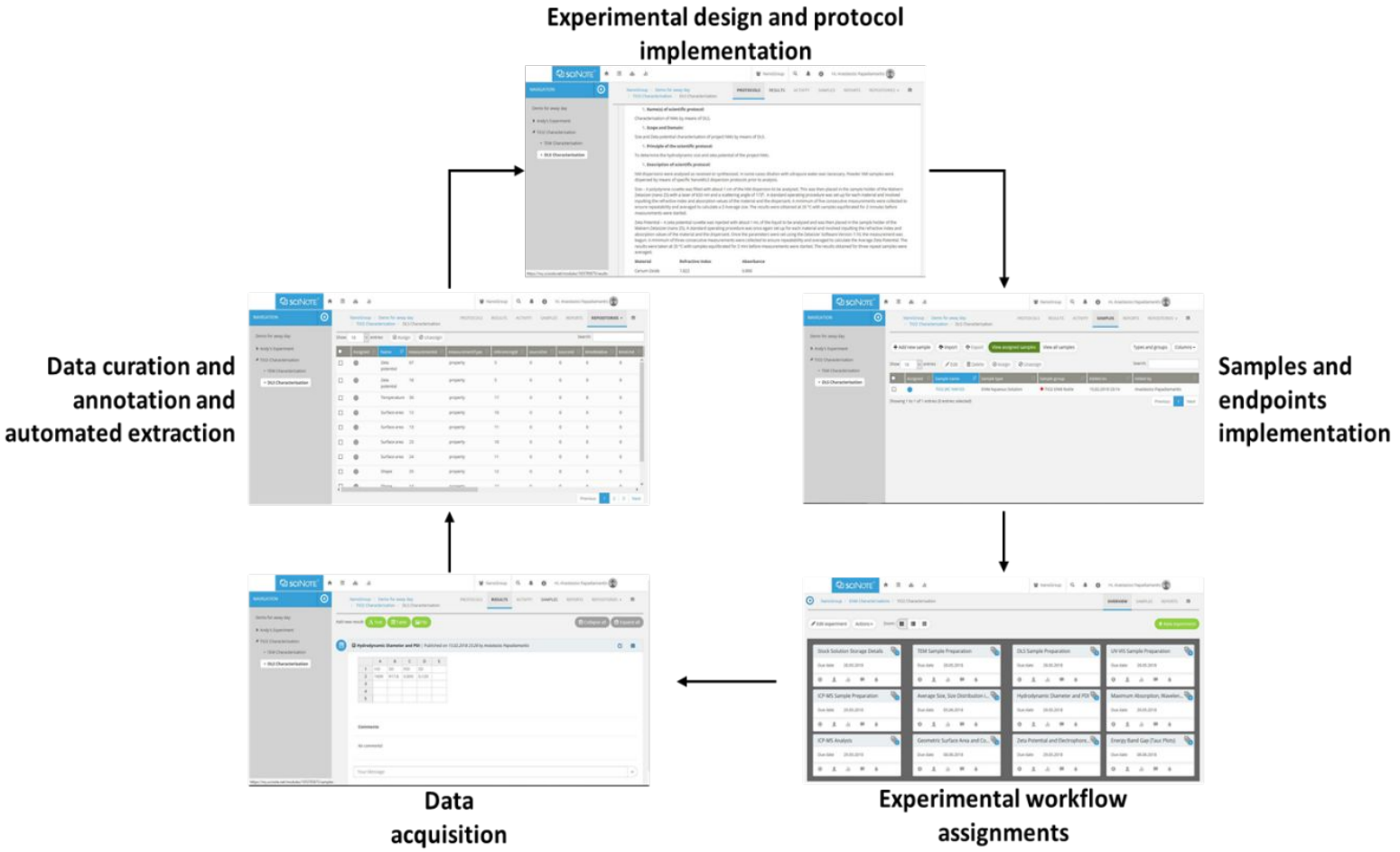
- The instance describes the lifecycle of nanomaterials
- Flexible and dynamic template able to include different types of materials including all metadata

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**

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Annotation

Ontology development and integration

OpenRiskNet/NanoCommons ontology meeting

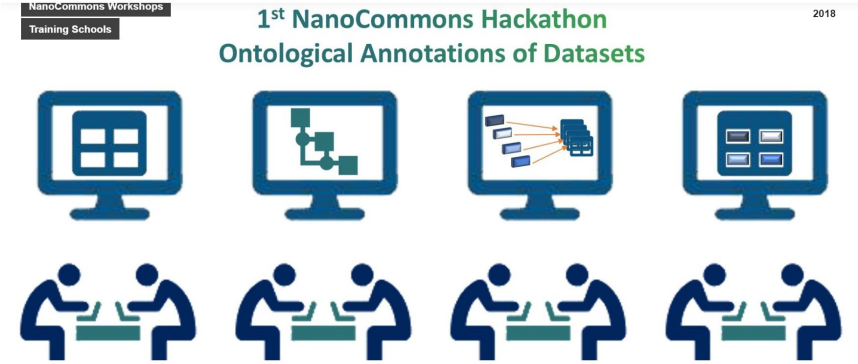
Workshop, Hackathon (co-organized by OpenRiskNet)
13 – 14 Dec 2018 / Brussels, BE

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.



The 1st NanoCommons Hackathon on "Ontological Annotation of Datasets" is co-organised by H2020 projects NanoCommons and OpenRiskNet. The hackathon will take place during the afternoon on 9 October 2018 in conjunction with the next NanoCommons Consortium Meeting (8-9 October 2018) and the OpenTox Euro Conference (8-11 October 2018) in Athens, Greece.

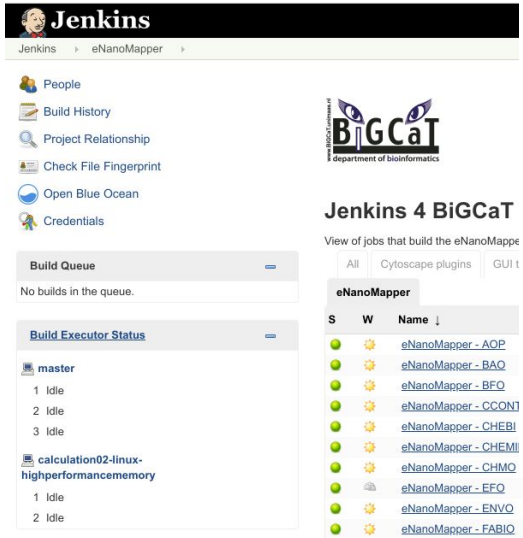
Available terms often not specific enough or misleading

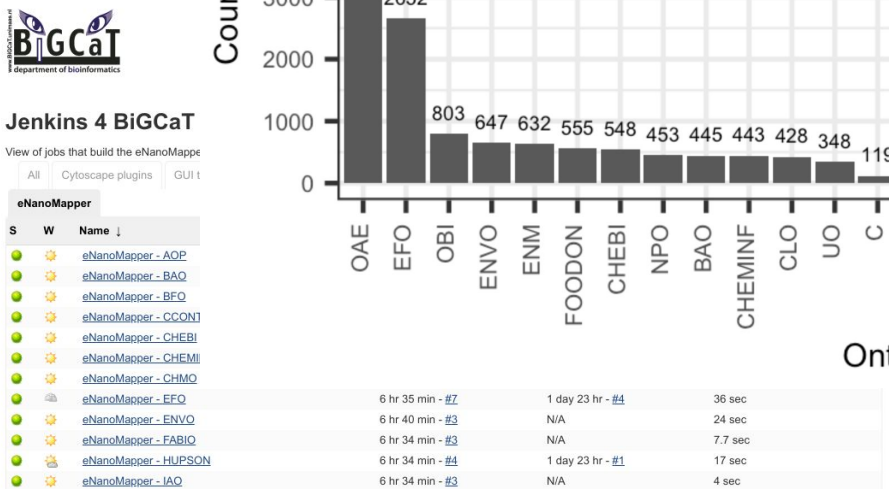
→ More complex terms needed

→ Better definitions

→ More training

Ontology development and integration





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

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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.

Endpoint: http://www.bioassayontology.org/bao#BAO_0000179

Technique: http://purl.bioontology.org/ontology/npo#NPO_1405

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

Measurement

Endpoints	
Technique	
Type of raw data produced	– BET Specific Surface Area using 5 isotherm data points at the adsorption branch of the isotherm within 0.05 ≤ p/po ≤ 0.2 – C-constant – p/p0 – isotherm correlation coefficient
Measurement quality parameters	last adsorption isotherm data point taken at p/po – *common setting:* 0.2 first isotherm data point taken at p/po – *common setting:* 0.01- 0.05
Phase in which the measurement is performed	Powder

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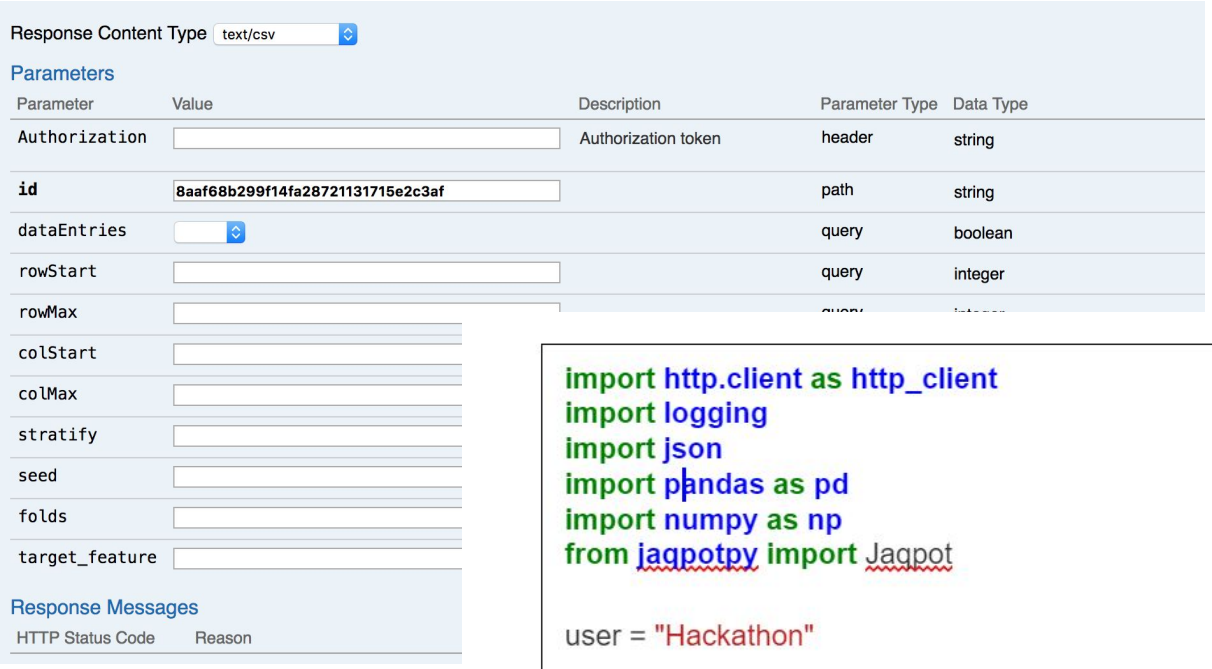
Links to other NanoCommons services and how to find relevant Transnational Access offerings

Tools for data search and retrieval: data APIs




```
import http.client as http_client
import logging
import json
import pandas as pd
import numpy as np
from jaqpotpy import Jaqpot

user = "Hackathon"

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

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

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

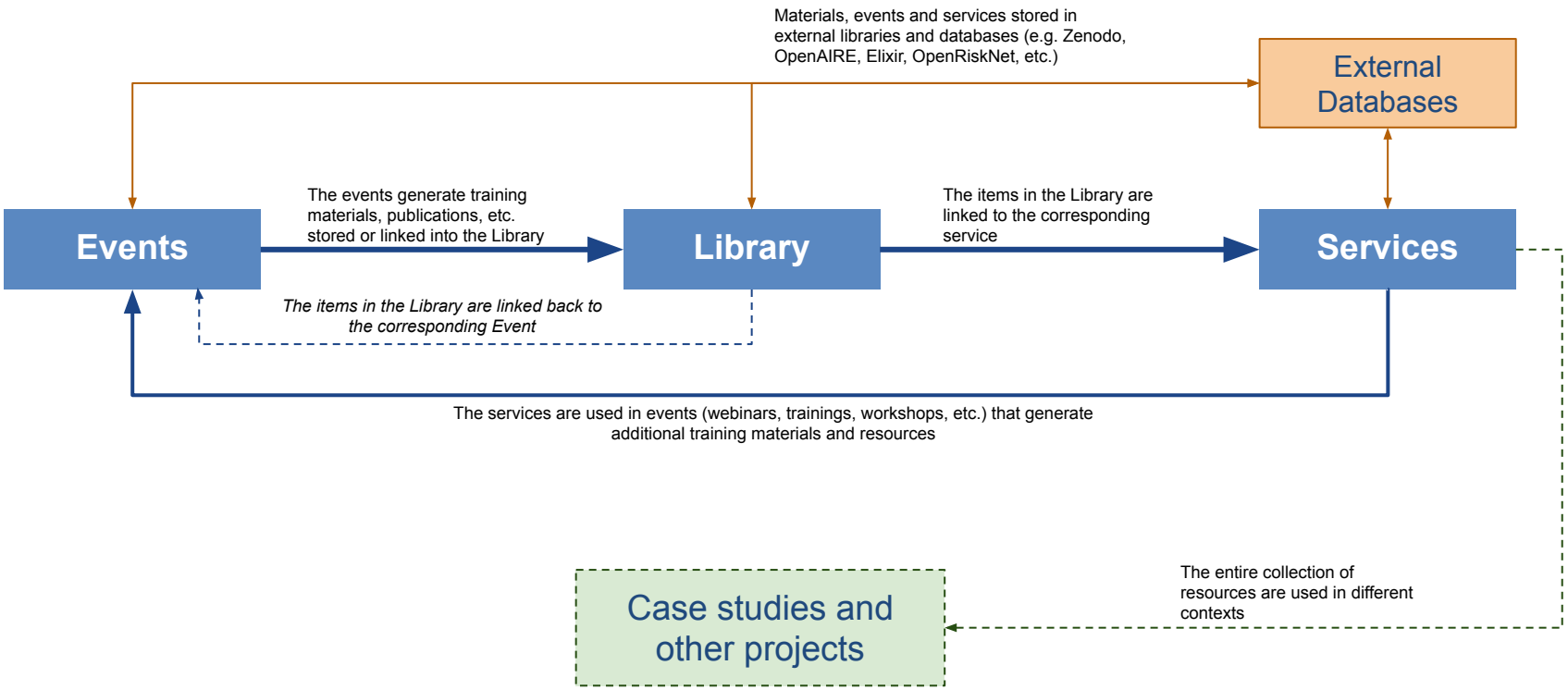
```
on...")
                =                    requests.get(url                +
Simple?name={}&password={}".format(user, pw),
es=proxies)
```

OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE

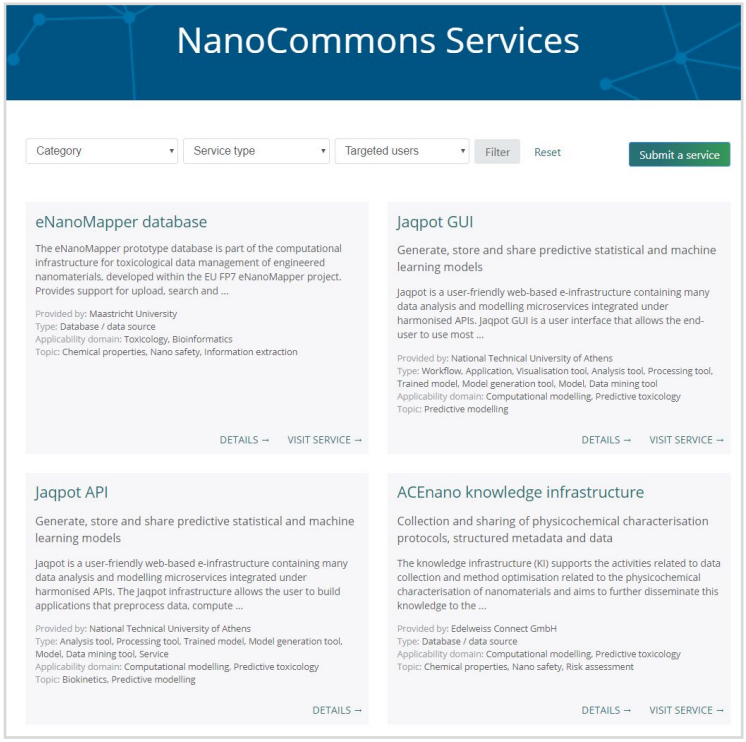
Service descriptions and discover service

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.)



- **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

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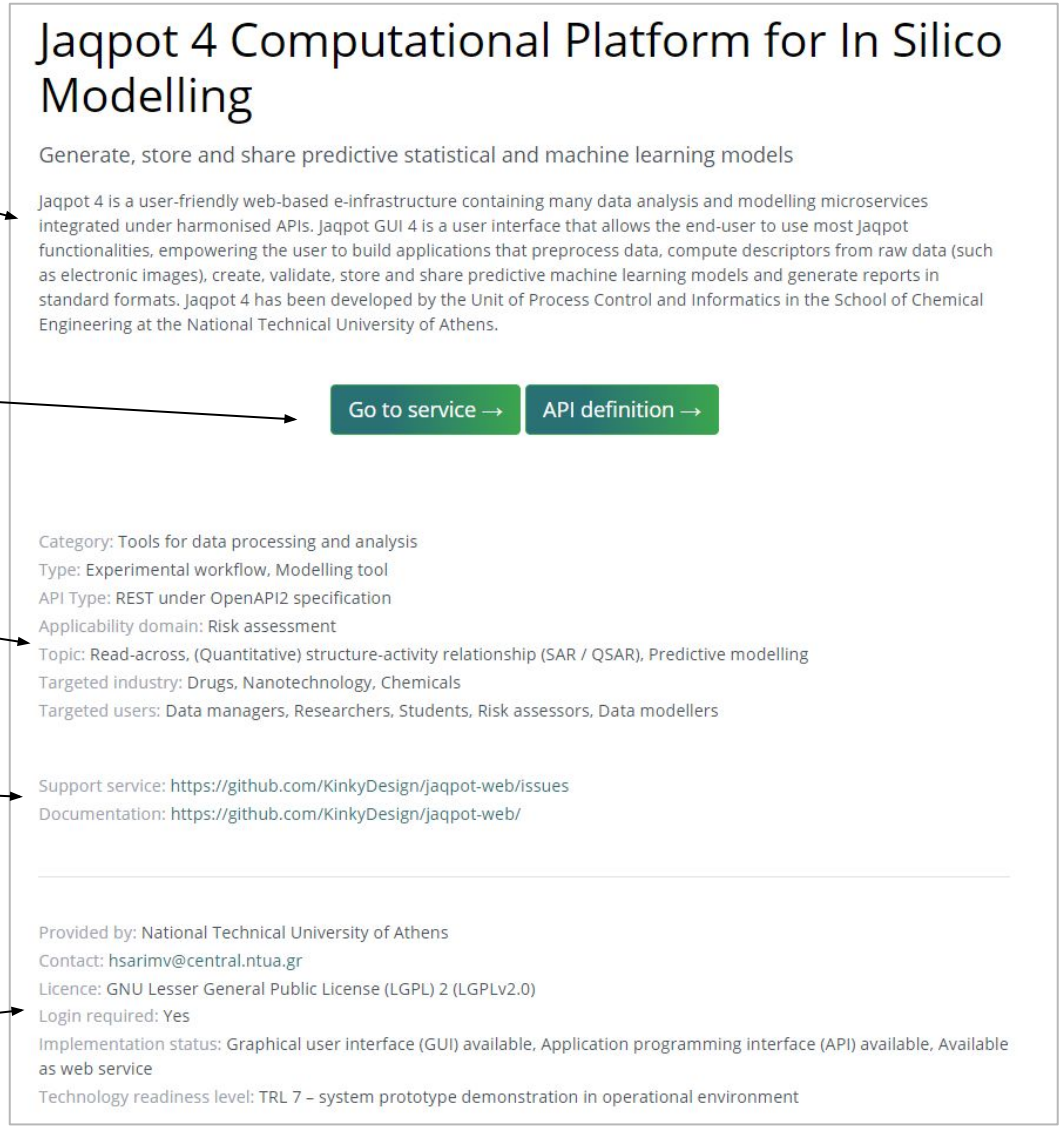
General description

Direct URLs to the service

Service identification

Training and user support

Contact and additional information on licence, TRLs, etc.



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Conclusion

Call to action

- 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
  - A.Papadiamantis@bham.ac.uk
  - I.Lynch@bham.ac.uk
- Visit 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!*

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Dieter Maier
BioMax Informatics AG

Joh Dokler, Lucian Farcal,
Maja Brajnik
Edelweiss Connect GmbH

Iseult Lynch, Tassos Papadiamantis
University of Birmingham

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

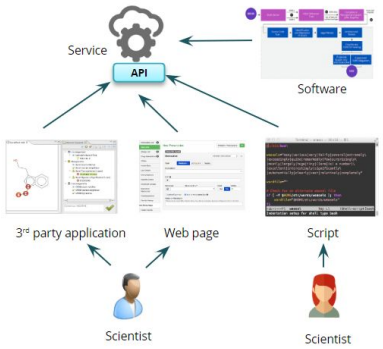
2016-2019 3 years project

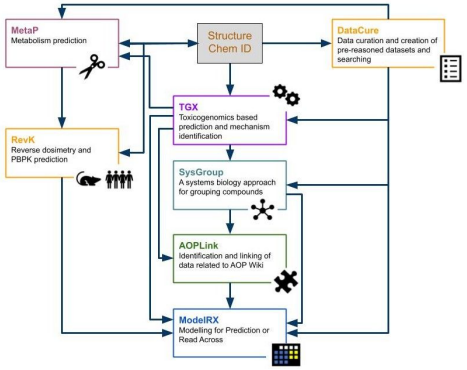
3 mil Total funding

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**:

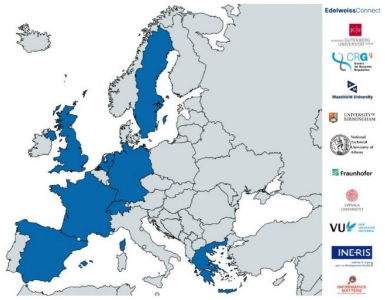
- **Harmonising** access to data and facilitating **interoperability** of software,
- Easily **deployable** to single computers, public and in-house cloud solutions,
- Addressing the needs of **industry and academic researchers, risk assessors and regulators.**

Final Workshop

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

23 - 24 October 2019
Amsterdam, Netherlands

https://openrisknet.org/events/



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)
P7 Fraunhofer Gesellschaft Zur Foerderung 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)

Publications & Training Resources
https://openrisknet.org/library/