



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

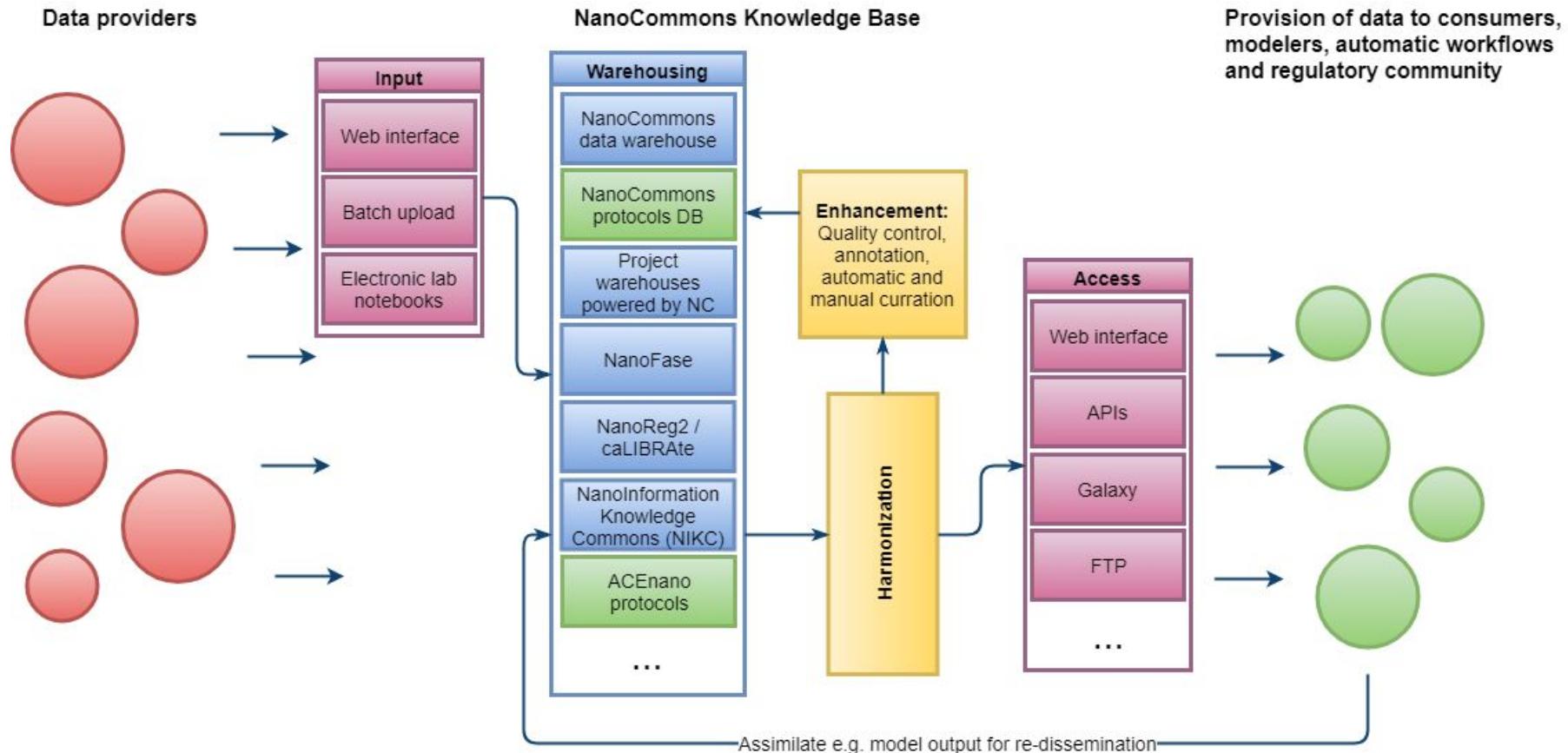
*NanoSafety Cluster week
Copenhagen, 9 October 2019*



Data Driven Innovation – Added Value



Scope of the data management tasks





Data management and sharing



NanoCommons
Nano-Knowledge Community

NanoCommons Knowledge Infrastructure



NanoCommons Platform

Search...

Folder (0) Collect Admin

Home News My Profile Help Help Desk Analysis Browse Ontologies Data Access Data Upload

Welcome to the NanoCommons Knowledge Base

Biomax INFORMATICS



Analysis



Data Access



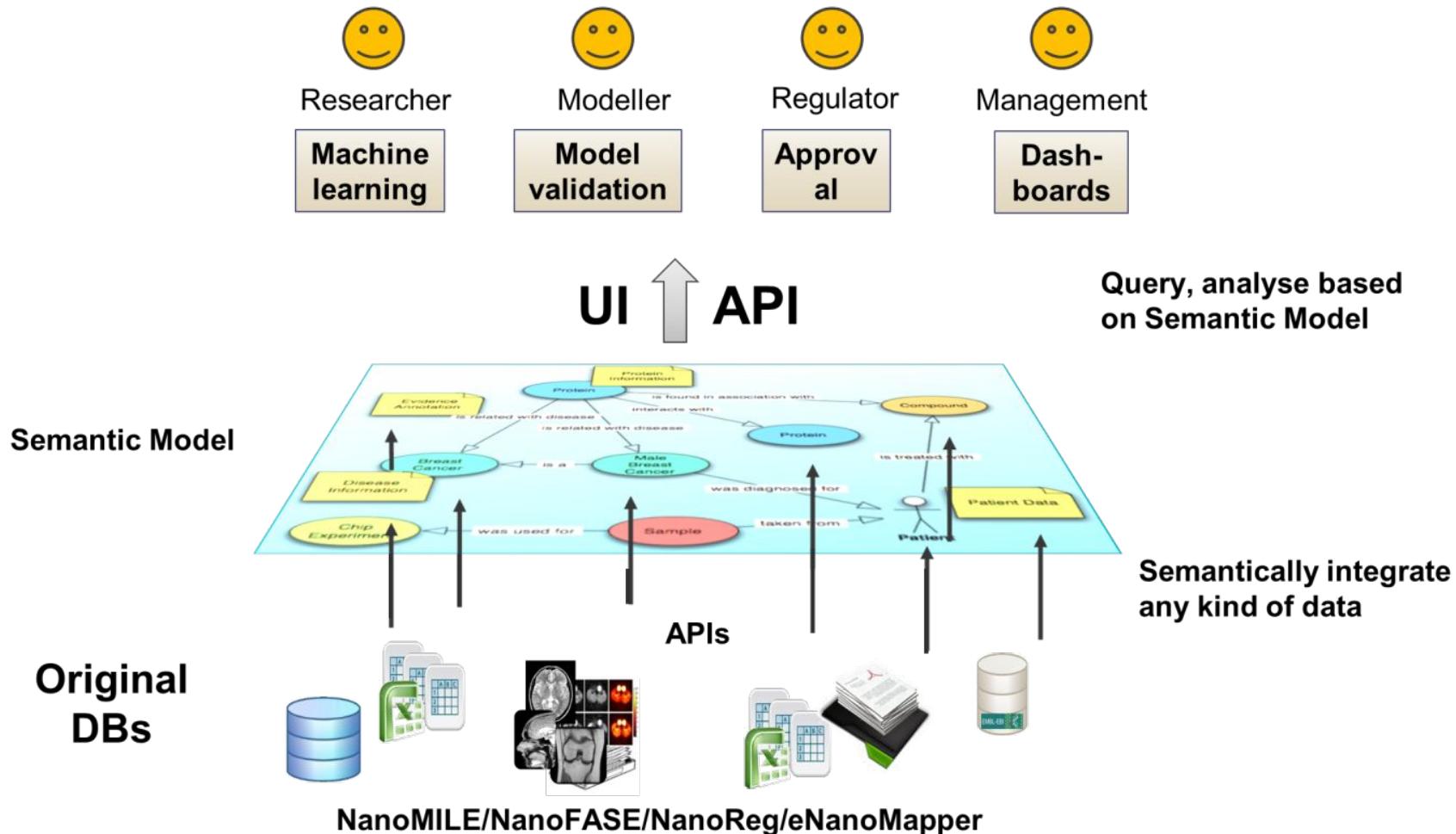
Upload Data



Ontologies



Why is it more than data warehousing?





NanoCommons data warehouse

NanoCommons Platform Export ▾ Folder ▾ (0) Collect ▾ Admin ▾

BioXM » Particles

Particle Characterisation

Characterisation data

Show/Hide ▾ Sort by ▾

Selected items: 0

| ID | Chemical Elements | Characterisation data | Samples | Aliquots | NanoFASE name | Designator |
|---|-------------------|-----------------------|--|---|-------------------------|----------------------|
| <input checked="" type="checkbox"/> 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 | JRC-CeO2-NM02101a002230 | JRC-CeO2-NM211-2163a |
| <input checked="" type="checkbox"/> NP00191 | Ce | NP00191 | JRC-CeO2-NM02101a002230 | JRC-CeO2-NM211-2163a | | |

View: General - NanoFASE - Instance

- + Search

| ID | Name | Instance ID | Time of Measure... | Time of Measur... | Medium | Sample | | Protocols | | | | | | |
|-------------|------------------------------|-------------|--------------------|-------------------|------------|----------------|----------------------|---------------|-------------------|------------------------|------------------|------------|-----------|------------|
| | | | | | | ID | Name | 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 | | | | | | | |
| IN000011703 | 01.001/1000_control | | control | 0.0 min | 0.0 min | SAMP_000000472 | MWCNT powder | | | | | | | |
| IN000011704 | 01.001/1000_I0 | I0 | | 0.0 min | 0.0 min | SAMP_000000464 | Released materials | | | | | | | |
| IN000011705 | 01.001/1000_I2 | I2 | | 200.0 min | 200.0 min | SAMP_000000473 | Released materials | | | | | | | |
| IN000011706 | 01.001/1000_I3 | I3 | | 0.0 min | 200.0 min | SAMP_000000465 | MWCNT-PP | 01.001/1000_3 | SEM-EDX analysis | ISM-6010 LV, JEOL Ltd. | | | | |
| IN000011707 | 01.001/1000_I4 | I4 | | 0.0 min | 200.0 min | SAMP_000000474 | MWCNT-PP | 01.001/1000_6 | Nanocomposite | (CoolSafe 100-9 PRO | | | | |
| IN000011708 | 01.001/1000_I5 | I5 | | 1000.0 min | 1200.0 min | SAMP_000000466 | Aged MWCNT-PP | 01.001/1000_4 | Weathering 200 h | 01.001/1000_1.0 | Climatic | climatic | | |
| IN000011709 | 01.001/1000_I6 | I6 | | 0.0 min | 1200.0 min | SAMP_000000475 | Aged MWCNT-PP | 01.001/1000_6 | Nanocomposite | (CoolSafe 100-9 PRO | | | | |
| IN000011710 | 01.001/1000_I7 | I7 | | 0.0 min | 1200.0 min | SAMP_000000467 | Milled aged MWCNT-PP | 01.001/1000_7 | recycling | 01.001/1000_1.0 | Polymer grinding | | | |
| IN000011708 | 01.001/1000_I5 | I5 | | 1000.0 min | 1200.0 min | SAMP_000000468 | Weathered recycled | 01.001/1000_3 | SEM-EDX analysis | ISM-6010 LV, JEOL Ltd. | | | | |
| IN000011709 | 01.001/1000_I6 | I6 | | 0.0 min | 1200.0 min | SAMP_000000476 | Weathered recycled | 01.001/1000_4 | Weathering 200 h | 01.001/1000_1.0 | Climatic | climatic | | |
| IN000011710 | 01.001/1000_I7 | I7 | | 0.0 min | 1200.0 min | SAMP_000000477 | Recycled MWCNT-PP | 01.001/1000_6 | Nanocomposite | (CoolSafe 100-9 PRO | | | | |
| IN000011708 | 01.001/1000_I5 | I5 | | 1000.0 min | 1200.0 min | SAMP_000000478 | Recycled MWCNT-PP | 01.001/1000_7 | recycling | 01.001/1000_1.0 | Polymer grinding | | | |
| IN000011709 | 01.001/1000_I6 | I6 | | 0.0 min | 1200.0 min | SAMP_000000469 | Weathered recycled | 01.001/1000_3 | SEM-EDX analysis | ISM-6010 LV, JEOL Ltd. | | | | |
| IN000011710 | 01.001/1000_I7 | I7 | | 0.0 min | 1200.0 min | SAMP_000000479 | Weathered recycled | 01.001/1000_4 | Weathering 200 h | 01.001/1000_1.0 | Climatic | climatic | | |
| IN000011708 | 01.001/1000_I5 | I5 | | 1000.0 min | 1200.0 min | SAMP_000000480 | Weathered recycled | 01.001/1000_5 | Weathering 1000 h | 01.001/1000_1.0 | Climatic | climatic | | |

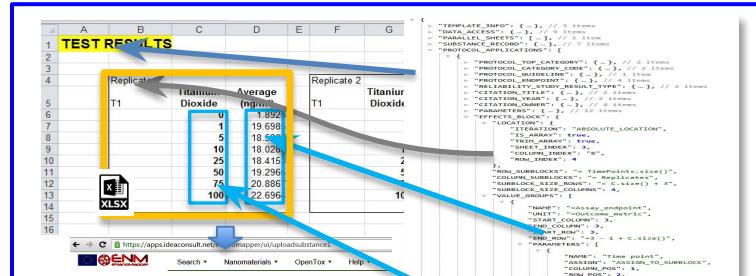
View: General - Instrument

- + Search

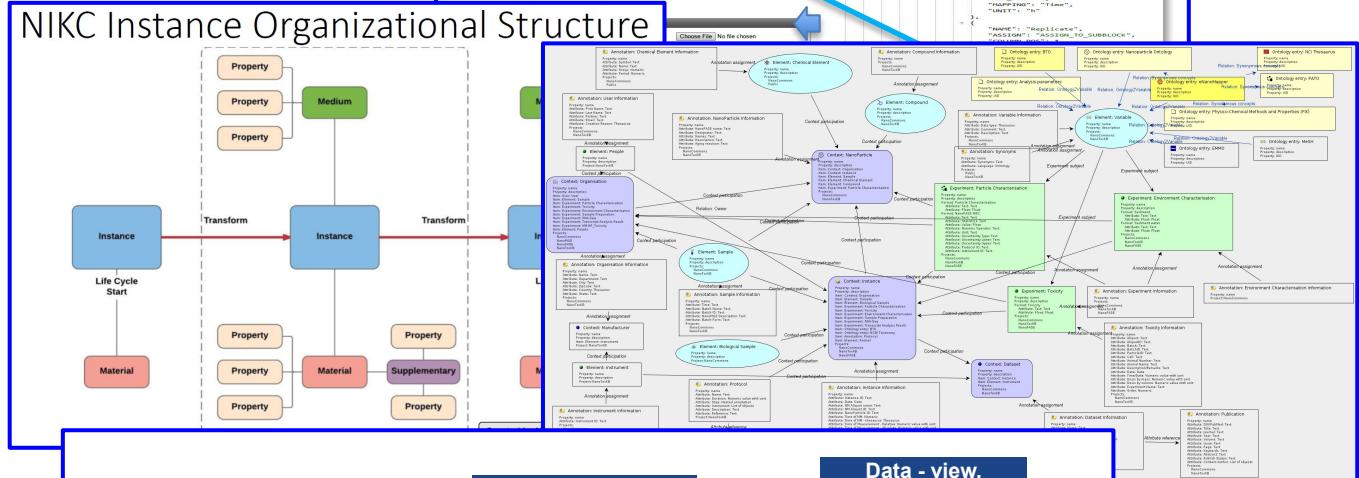
| Instrument | Manufacturer | Used for dataset |
|-----------------|----------------------|------------------|
| IEOL | IEOL | 01.001/1000 |
| D5000 | Bruker | 01.001/1000 |
| Agilent 7500 | Agilent Technologies | 01.001/1000 |
| CEM 1600W | MARS | 01.001/1000 |
| NRS 5 E | OVAN | 01.001/1000 |
| B500F FEG-SEM | IEOL | 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-1 8400 | Shimadzu | 01.001/1000 |
| ISM-6010 LV | IEOL | 01.001/1000 |

Data warehousing: external data sources

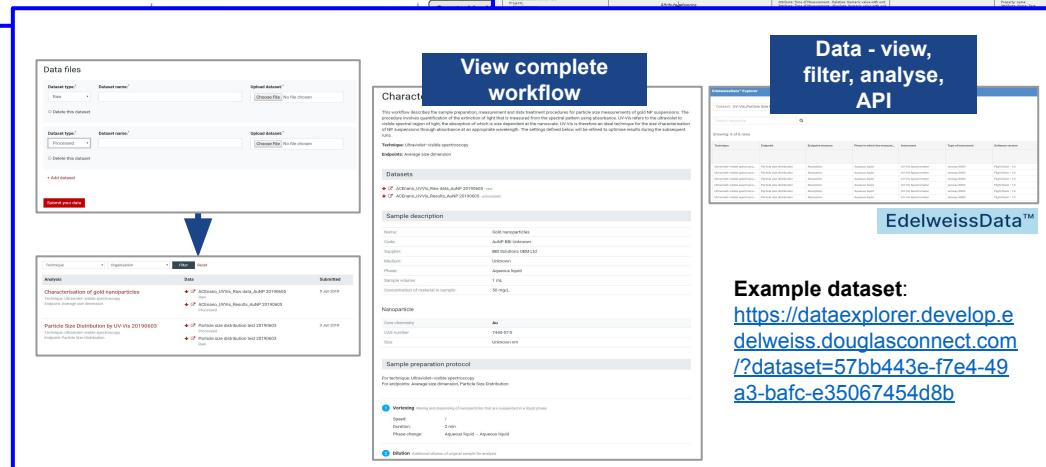
- eNanoMapper



- NIKC and NanoFase



- ACEnano



The figure shows the ACEnano Data Explorer interface. It includes sections for "Data files", "View complete workflow", and "Data - view, filter, analyse, API". The "Data files" section shows uploaded datasets and their descriptions. The "View complete workflow" section provides a timeline of experiments and their status. The "Data - view, filter, analyse, API" section displays a table of sample descriptions, including parameters like "Gold Nanoparticles", "Gold Nanoparticle", "Medium", "Phase", "Concentration of material in sample", "Nanoparticle", "Sample preparation protocol", and "Washing". At the bottom, there is a "EdelweissData™" logo and a link to an example dataset.

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



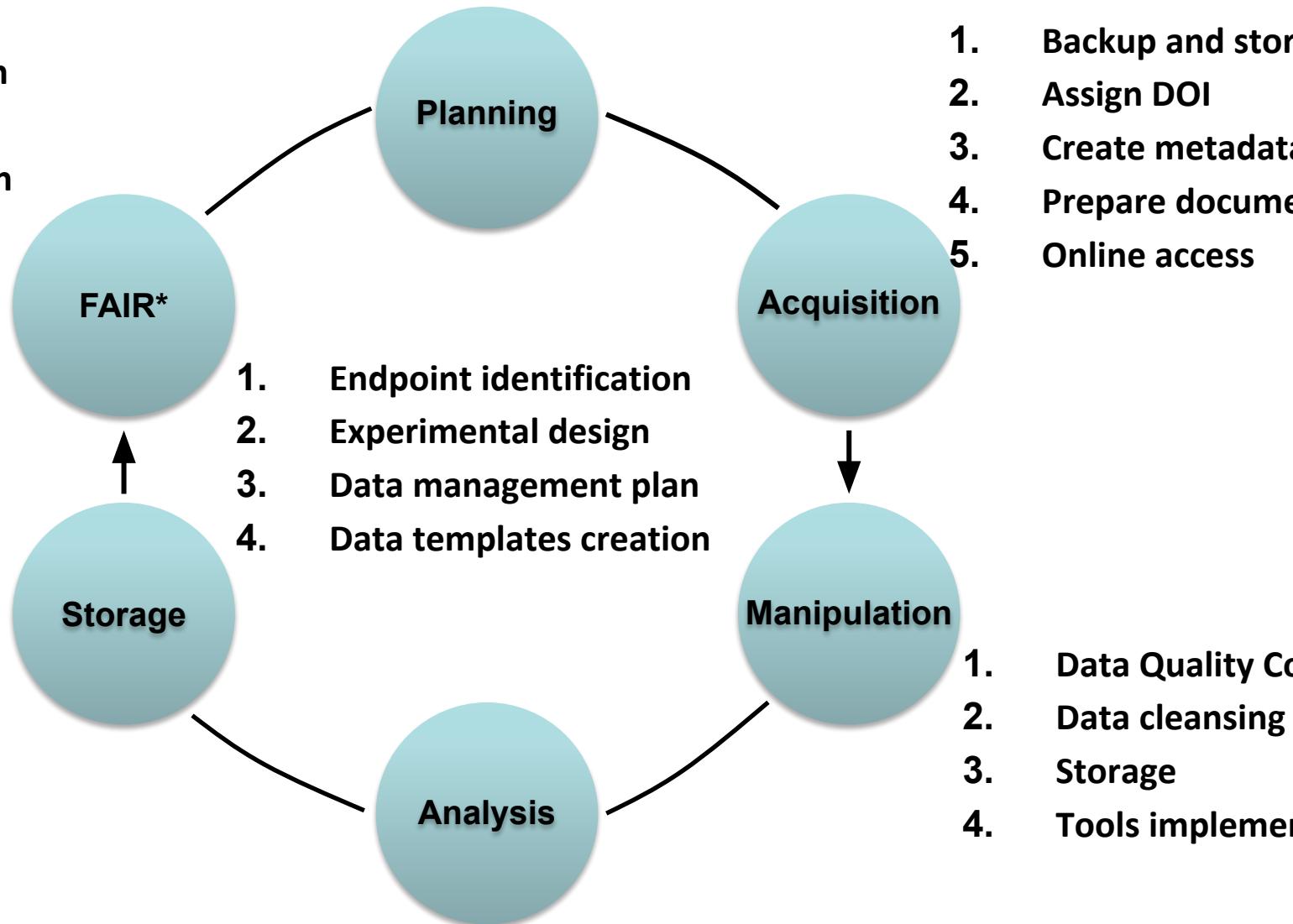
Data quality



Data management and data lifecycle

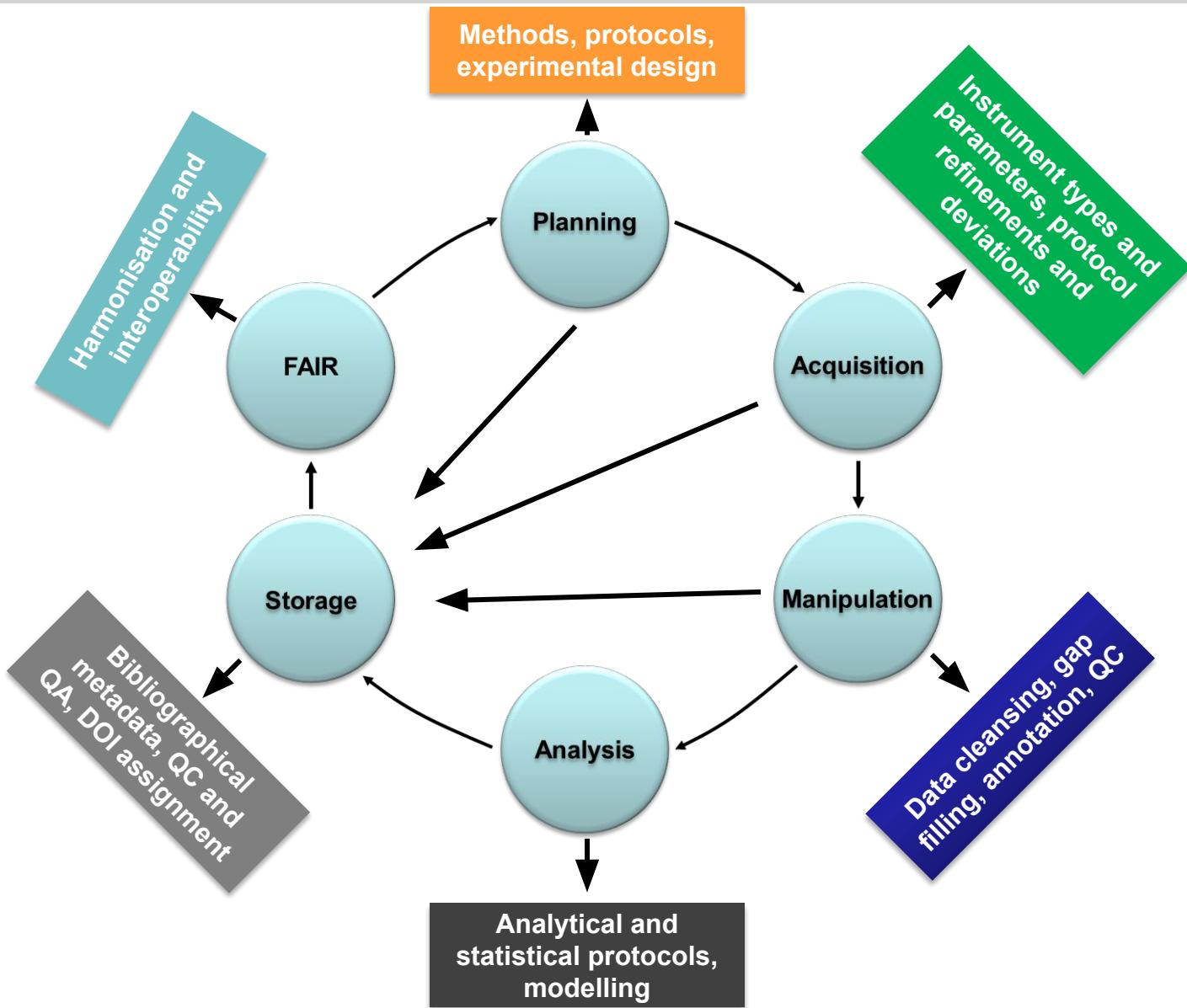
- Data acquisition
- Data curation
- Data digitisation

etation
QSARs/Omics
tputs



*Findable, Accessible, Interoperable, Reusable

Data management, data lifecycle & metadata





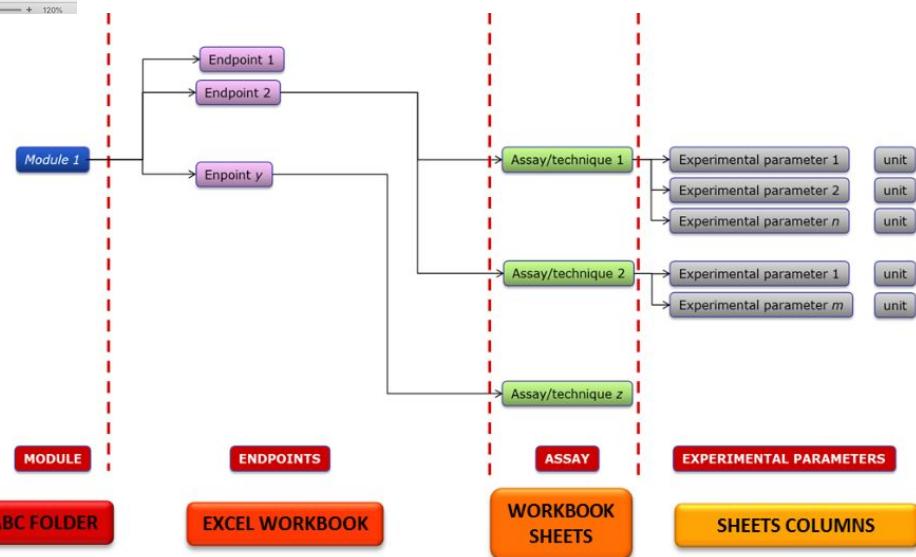
Can we harmonize data capturing?

| datasetid | instance | registry number | Material | Medium | measurementType | parameter | inheritId | parameterDescription | parameterdatatype | parameterText | parar |
|-------------|------------------|-----------------|-------------------|----------|----------------------------|--------------------------|-----------|----------------------|-------------------|----------------------------------|-------|
| 01.001/1000 | Stock dispersion | Envirox CeO2 NP | Water | property | CeO2 concentration | Reported by Experimenter | | | | mean | |
| 01.001/1000 | Stock dispersion | Envirox CeO2 NP | Water | property | mean primary particle size | Reported by Experimenter | | | | mean | |
| 01.001/1000 | ID | | Sewage sludge | property | Ce concentration | Reported by Experimenter | | | | mean | |
| 01.001/1000 | ID | | Sewage sludge | Property | Total solids | Reported by Experimenter | | | | mean | |
| 01.001/1000 | I1 | | Sewage sludge | Property | Amount | Reported by Experimenter | | Numeric | | Amount of Ce added to the sludge | |
| 01.001/1000 | I1 | Envirox CeO2 NP | Sewage sludge | Property | Mass | Reported by Experimenter | | | | | |
| 01.001/1000 | I2 | | Dry sewage sludge | property | Ce concentration | Reported by Experimenter | | | | mean | |
| 01.001/1000 | I2 | | Dry sewage sludge | property | Ash content | Reported by Experimenter | | | | | |
| 01.001/1000 | I2 | | Dry sewage sludge | Property | Total carbon | Reported by Experimenter | | Numeric | | | |
| 01.001/1000 | I2 | Envirox CeO2 NP | Dry sewage sludge | property | XAS | Reported by Experimenter | | | | Data at Eawag | |
| 01.001/1000 | I3 | | Fly Ash | property | Mass | Reported by Experimenter | | | | | |
| 01.001/1000 | I3 | | Fly Ash | property | Ce concentration | Reported by Experimenter | | | | mean | |
| 01.001/1000 | I3 | | Fly Ash | Property | Total carbon | Reported by Experimenter | | Numeric | | | |
| 01.001/1000 | I3 | Envirox CeO2 NP | Fly Ash | property | XAS | Reported by Experimenter | | | | Data at Eawag | |
| 01.001/1000 | I3 | Envirox CeO2 NP | Fly Ash | property | TEM | Reported by Experimenter | | | | Data at Eawag | |
| 01.001/1000 | I4 | | Bottom ash | property | Mass | Reported by Experimenter | | | | | |
| 01.001/1000 | I4 | | Bottom ash | property | Ce concentration | Reported by Experimenter | | | | mean | |
| 01.001/1000 | I4 | | Bottom ash | Property | Total carbon | Reported by Experimenter | | Numeric | | | |
| 01.001/1000 | Stock dispersion | SkySprings CeO2 | Water | property | CeO2 concentration | Reported by Experimenter | | | | mean | |
| 01.001/1000 | Stock dispersion | SkySprings CeO2 | Water | property | mean primary particle size | Reported by Experimenter | | | | mean | |

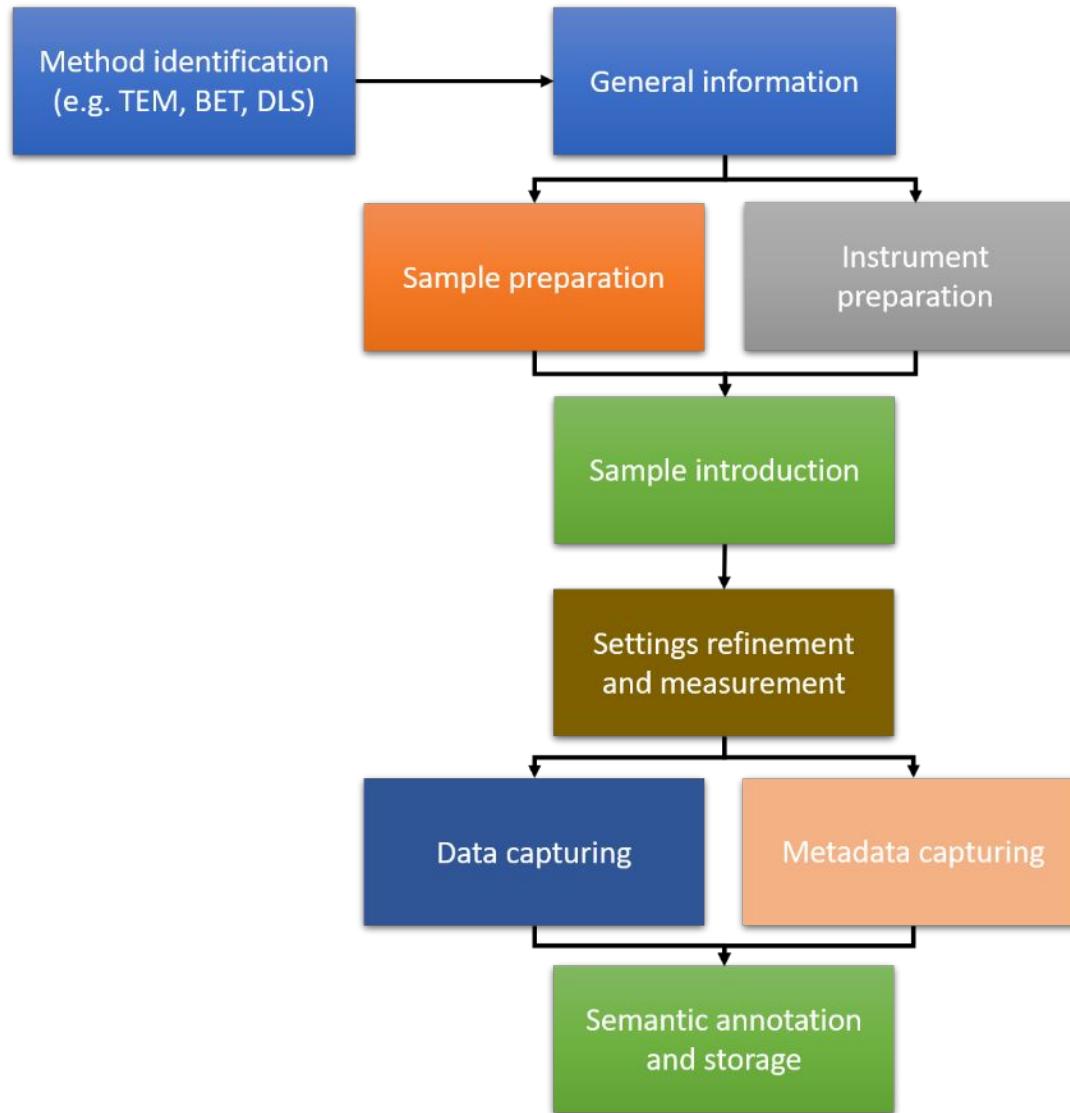
NIKC

- Evaluation of data capturing templates.

NanoREG templates



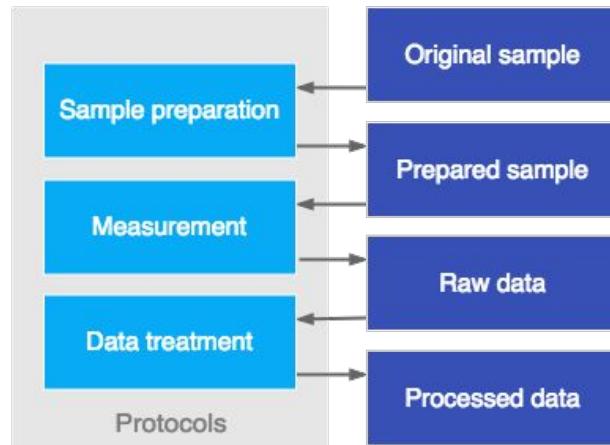
Protocols capturing workflow





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 unit:

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 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:^{*}

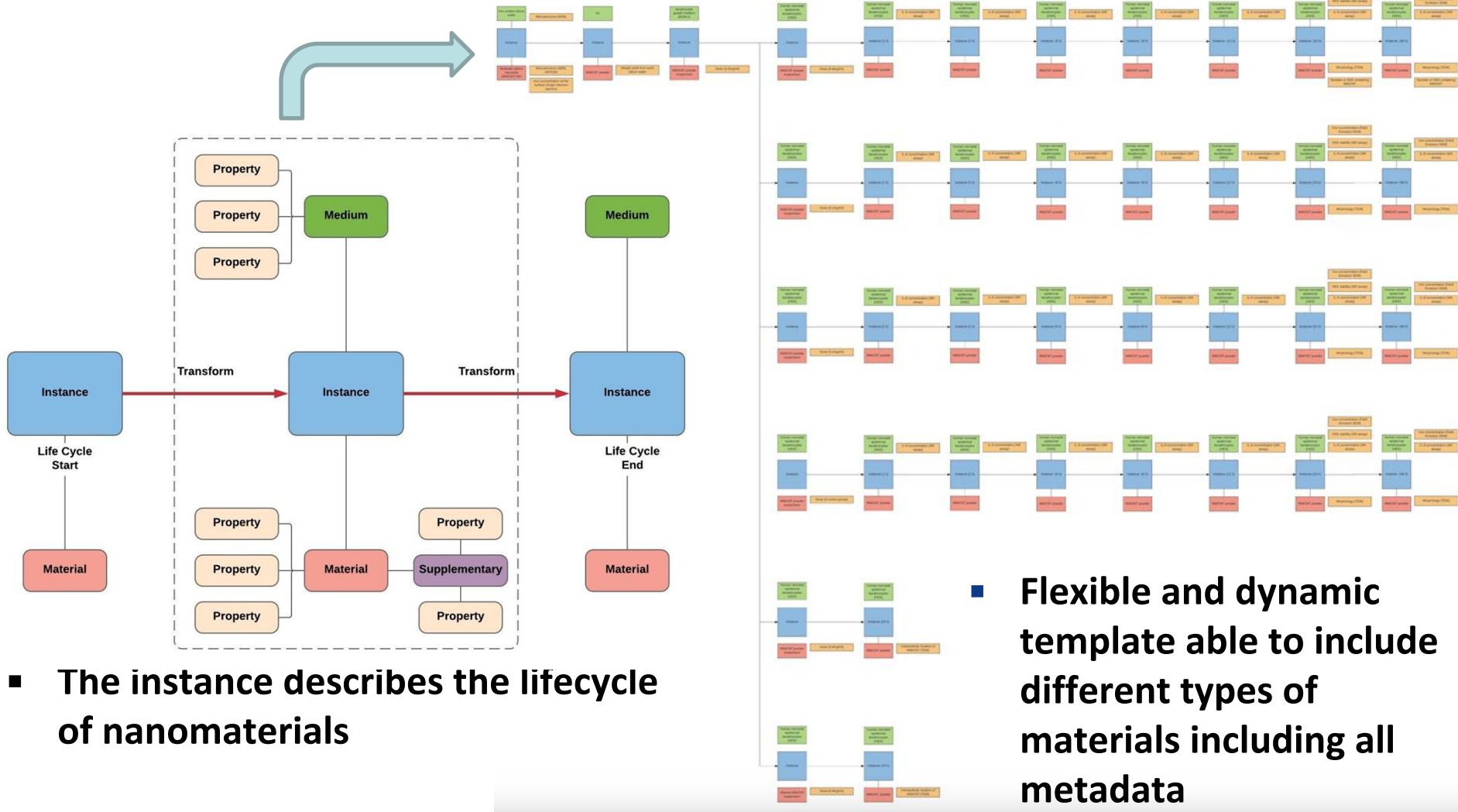
Common setting:

Units:

+ Add another quality parameter

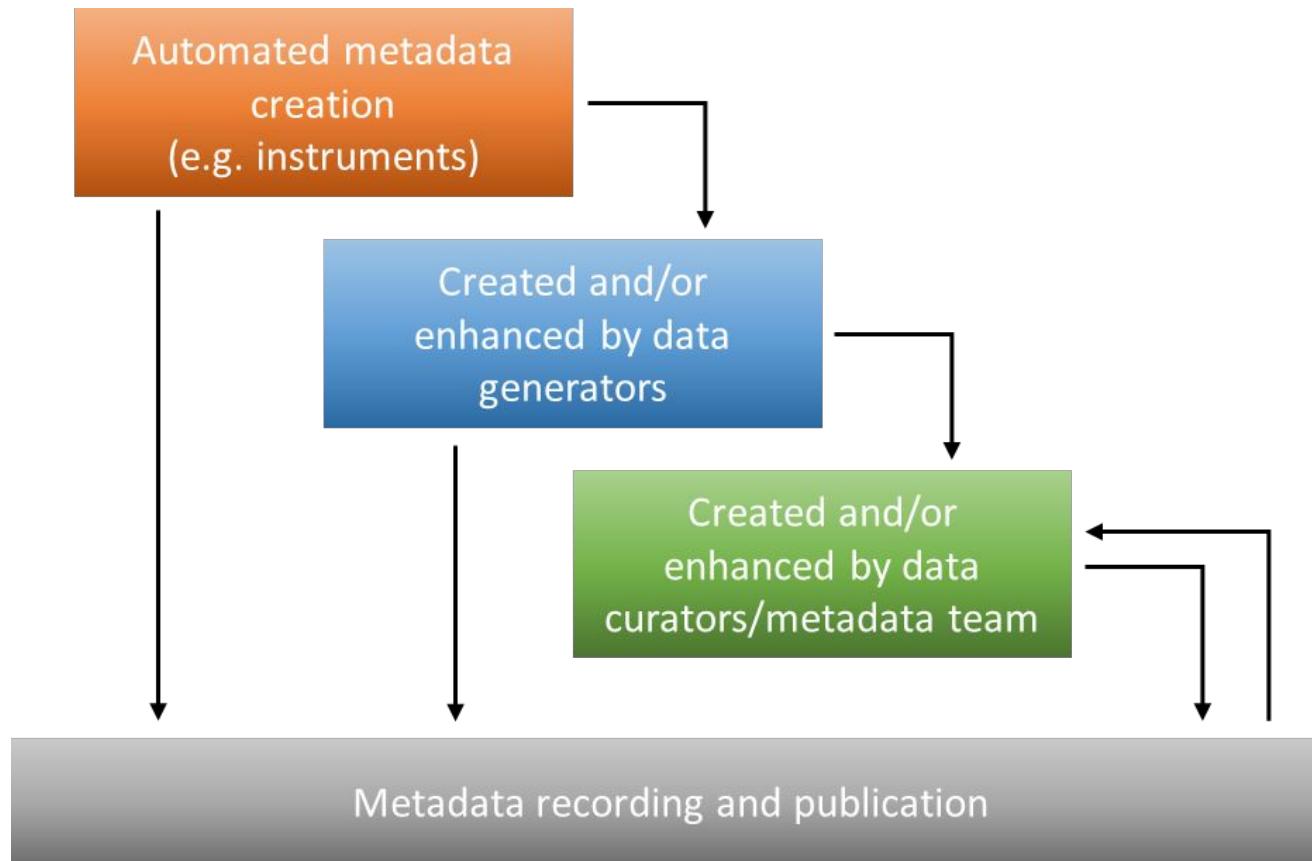
Continue to next step

How to deal with different life cycle states?





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**



NanoCommons
Nano-Knowledge Community

Annotation

Ontology development and integration

OpenRiskNet/NanoCommons ontology meeting

Workshop, Hackathon (co-organized by OpenRiskNet)

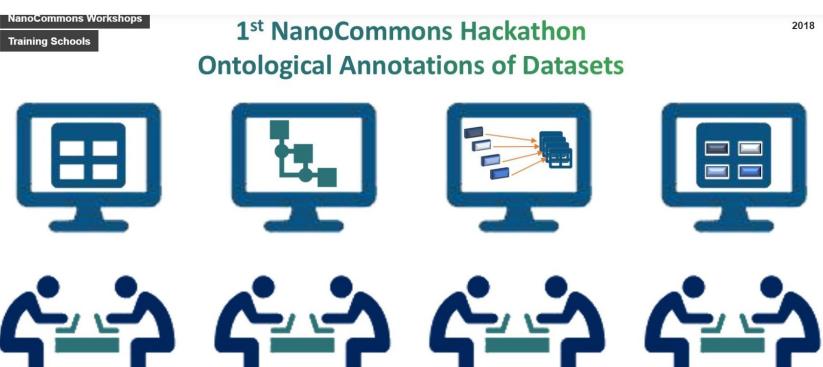
13 – 14 Dec 2018 / Brussels, BE

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.

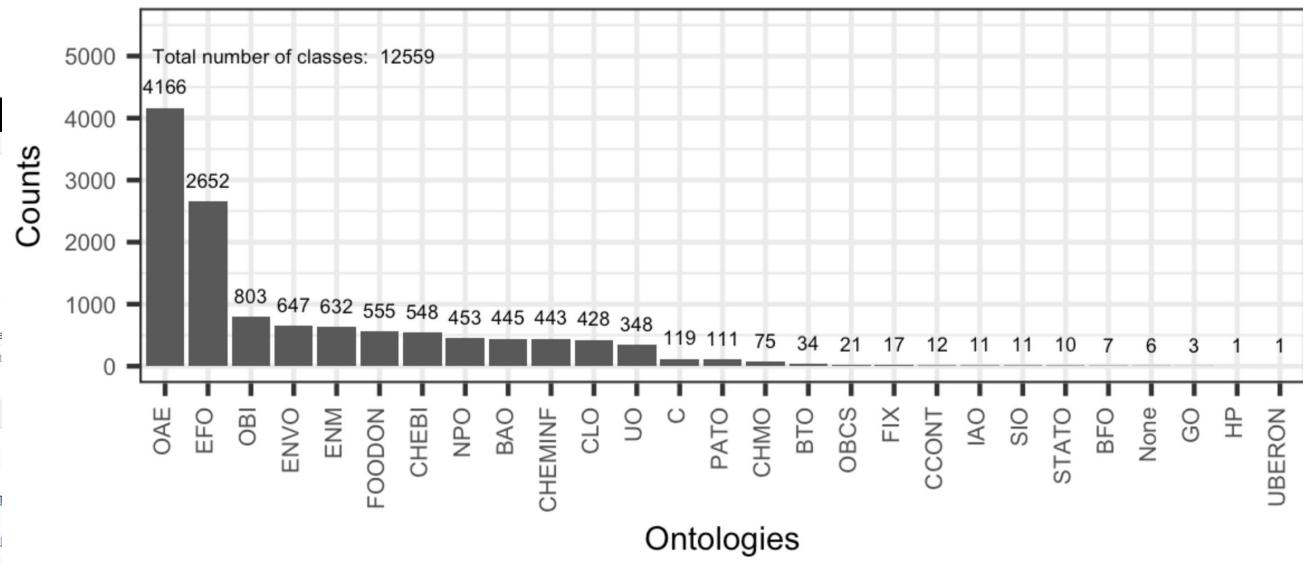
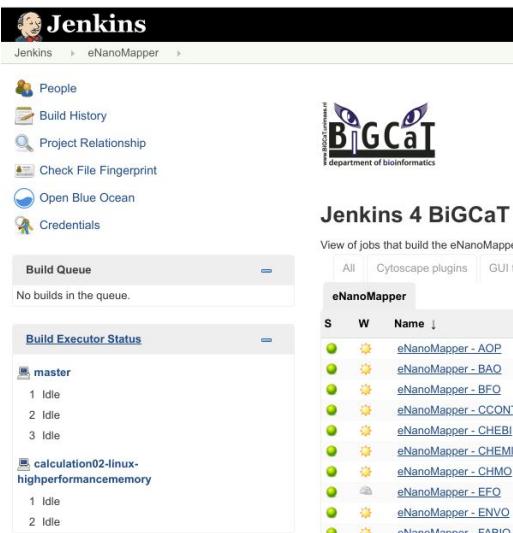


Available terms often not specific enough or misleading

- More complex terms needed
- Better definitions
- More training

Ontology development and integration

eNanoMapper ontologies

Jenkins 4 BiGCAT

View of jobs that build the eNanoMapper

Build Queue: All Cytoscape plugins GUI t

Build Executor Status:

- master: 1 Idle, 2 Idle, 3 Idle
- calculation02-linux-highperformancememory: 1 Idle, 2 Idle

eNanoMapper

| S | W | Name ↓ |
|---|---|----------------------|
| ● | ● | eNanoMapper - AOP |
| ● | ● | eNanoMapper - BAO |
| ● | ● | eNanoMapper - BFO |
| ● | ● | eNanoMapper - CCON1 |
| ● | ● | eNanoMapper - CHEBI |
| ● | ● | eNanoMapper - CHEMI |
| ● | ● | eNanoMapper - CHMO |
| ● | ● | eNanoMapper - EFO |
| ● | ● | eNanoMapper - ENVO |
| ● | ● | eNanoMapper - FABIO |
| ● | ● | eNanoMapper - HUPSON |
| ● | ● | eNanoMapper - IAO |

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

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

Endpoints

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

Technique

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="8aaef68b299f14fa28721131715e2c3af"/> | | path | string |
| dataEntries | <input type="checkbox"/> | | 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 | integer |
| seed | <input type="text"/> | | query | integer |
| folds | <input type="text"/> | | query | integer |
| target_feature | <input type="text"/> | | query | string |

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 jaqpotpy import Jaqpot

user = "Hackathon"

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

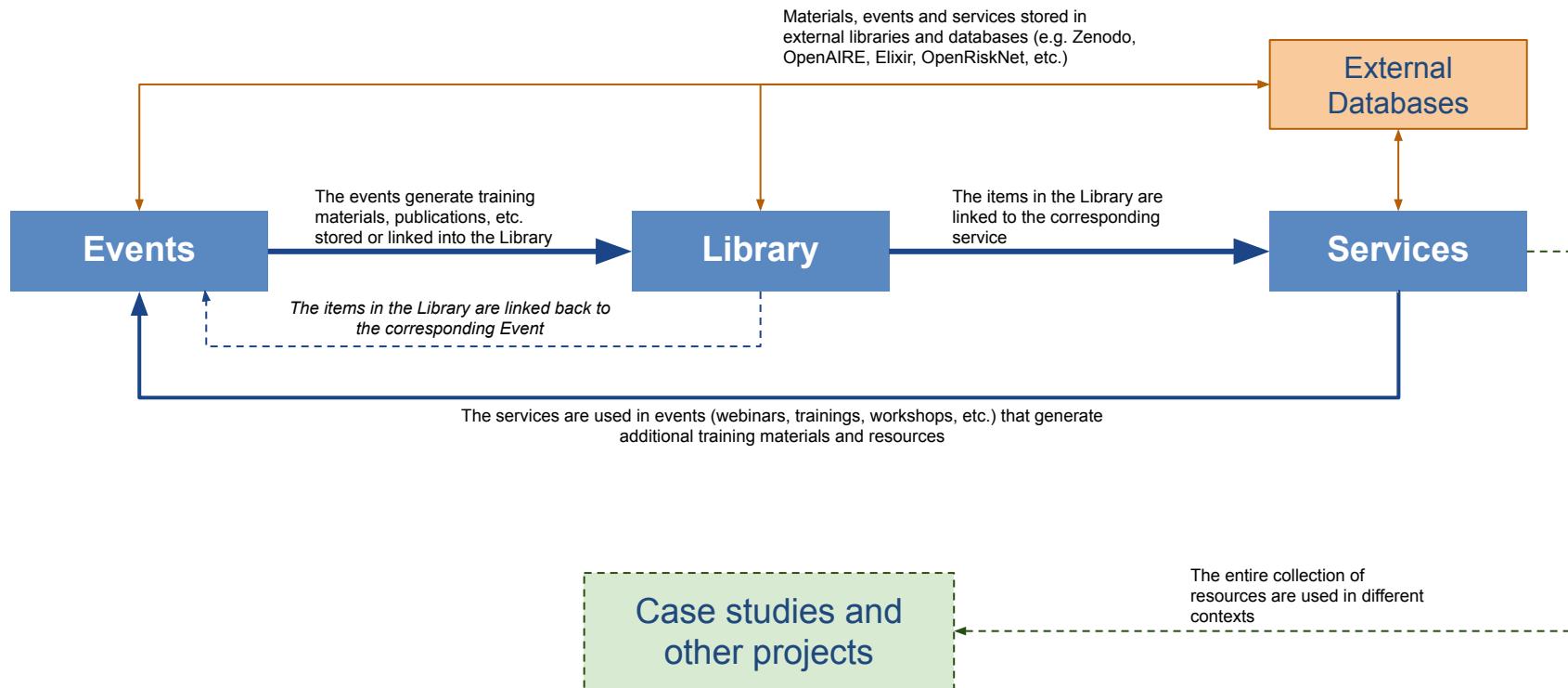
url = "https://ssl.biomax.de/nanocommons/bioxm/rest/api"

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

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

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 catalogue interface. At the top, there are search filters for Category, Service type, Targeted users, and a 'Submit a service' button. Below the filters, four service cards are displayed:

- eNanoMapper database**: Provided by Maastricht University. Type: Database / data source. Applicability domain: Toxicology, Bioinformatics. Topic: Chemical properties, Nano safety, Information extraction.
- Jaqpot GUI**: 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.
- Jaqpot API**: Provided by Edelweiss Connect GmbH. 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 ...

Each service card has 'DETAILS →' and 'VISIT SERVICE →' buttons 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

General description

Jaqpot 4 Computational Platform for In Silico Modelling

Generate, store and share predictive statistical and machine learning models

Jaqpot 4 is a user-friendly web-based e-infrastructure containing many data analysis and modelling microservices integrated under harmonised APIs. Jaqpot GUI 4 is a user interface that allows the end-user to use most Jaqpot functionalities, empowering the user to build applications that preprocess data, compute descriptors from raw data (such as electronic images), create, validate, store and share predictive machine learning models and generate reports in standard formats. Jaqpot 4 has been developed by the Unit of Process Control and Informatics in the School of Chemical Engineering at the National Technical University of Athens.

Direct URLs to the service

[Go to service →](#) [API definition →](#)

Service identification

Category: Tools for data processing and analysis

Type: Experimental workflow, Modelling tool

API Type: REST under OpenAPI2 specification

Applicability domain: Risk assessment

Topic: Read-across, (Quantitative) structure-activity relationship (SAR / QSAR), Predictive modelling

Targeted industry: Drugs, Nanotechnology, Chemicals

Targeted users: Data managers, Researchers, Students, Risk assessors, Data modellers

Training and user support

Support service: <https://github.com/KinkyDesign/jaqpot-web/issues>

Documentation: <https://github.com/KinkyDesign/jaqpot-web/>

Contact and additional information on licence, TRLs, etc.

Provided by: National Technical University of Athens

Contact: hsarimv@central.ntua.gr

Licence: GNU Lesser General Public License (LGPL) 2 (LGPLv2.0)

Login required: Yes

Implementation status: Graphical user interface (GUI) available, Application programming interface (API) available, Available as web service

Technology readiness level: TRL 7 – system prototype demonstration in operational environment



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

“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

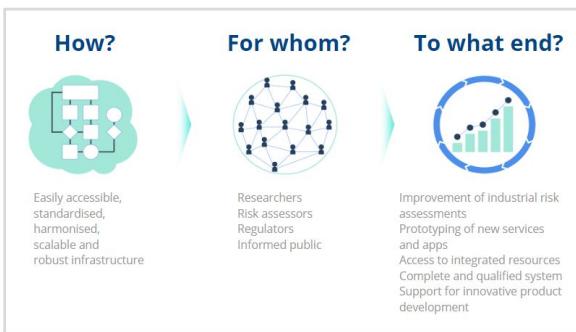
Iseult Lynch, Tassos Papadiamantis
University of Birmingham

Joh Dokler, Lucian Farcal,
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)



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**.

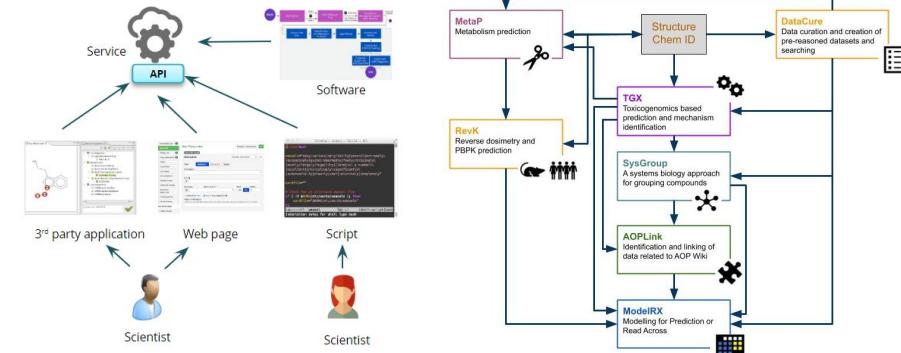


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