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

Adoption of OpenRisknet solutions by **NanoSafety community** and **NanoCommons** infrastructure

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OpenRiskNet Final Conference
*Amsterdam, 23-24 October 2019*

The idea

- **Nanotechnologies** are a major area of **investment & growth for the European economy**

- Knowledge and data remain fragmented and inaccessible **hampering progress**

- R**ead-across approaches are currently absent for NMs**, but would reduce the cost of nanosafety research and regulation dramatically

- **NanoCommons** is **creating an e-infrastructure** for reproducible science, **enhancing data integration & enabling nanoinformatics workflows** to address these gaps.
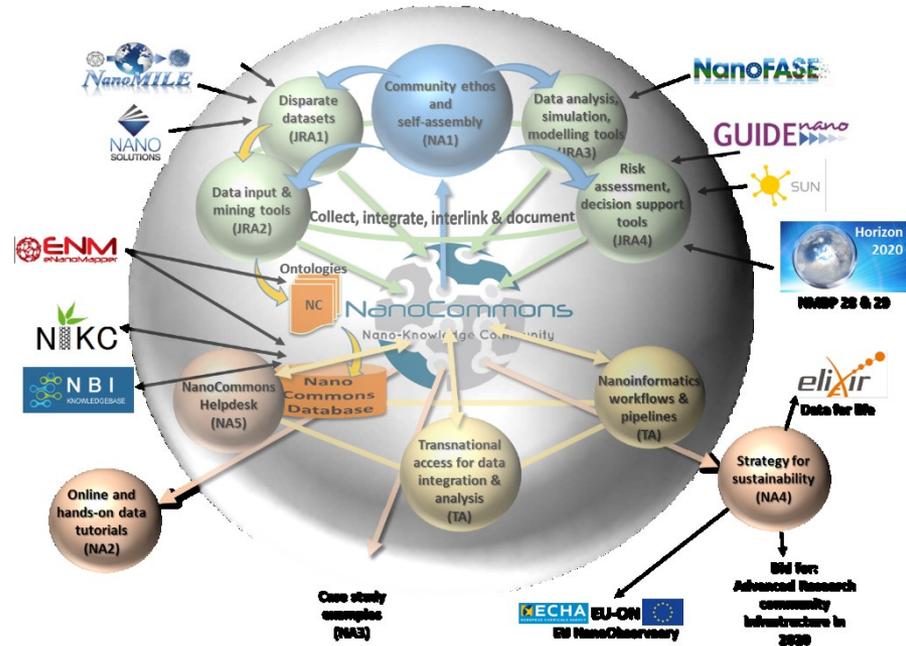
The approach

- Facilitate **identification** of potential **NM-related risks**

- Enable '**safe-by-design**' approaches

- **Support regulatory decision making** by ensuring data exploitation to assess "sameness", allow read-across

- Create a **FAIR data ecosystem** for data integration, sharing, enrichment and **full exploitation**;

- Enhance **public and expert engagement** through open debate on the benefits, risks and safe use of nanotechnology.
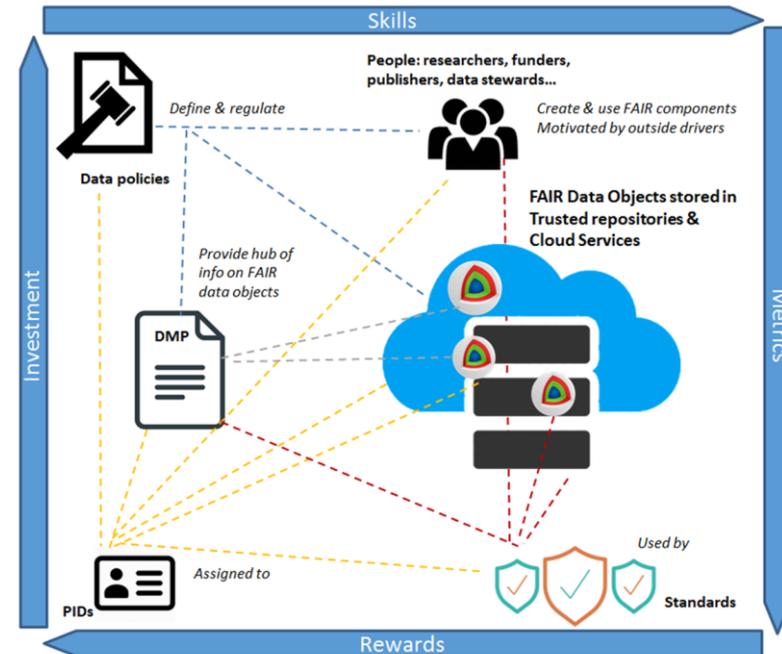
What's special about nanomaterials?
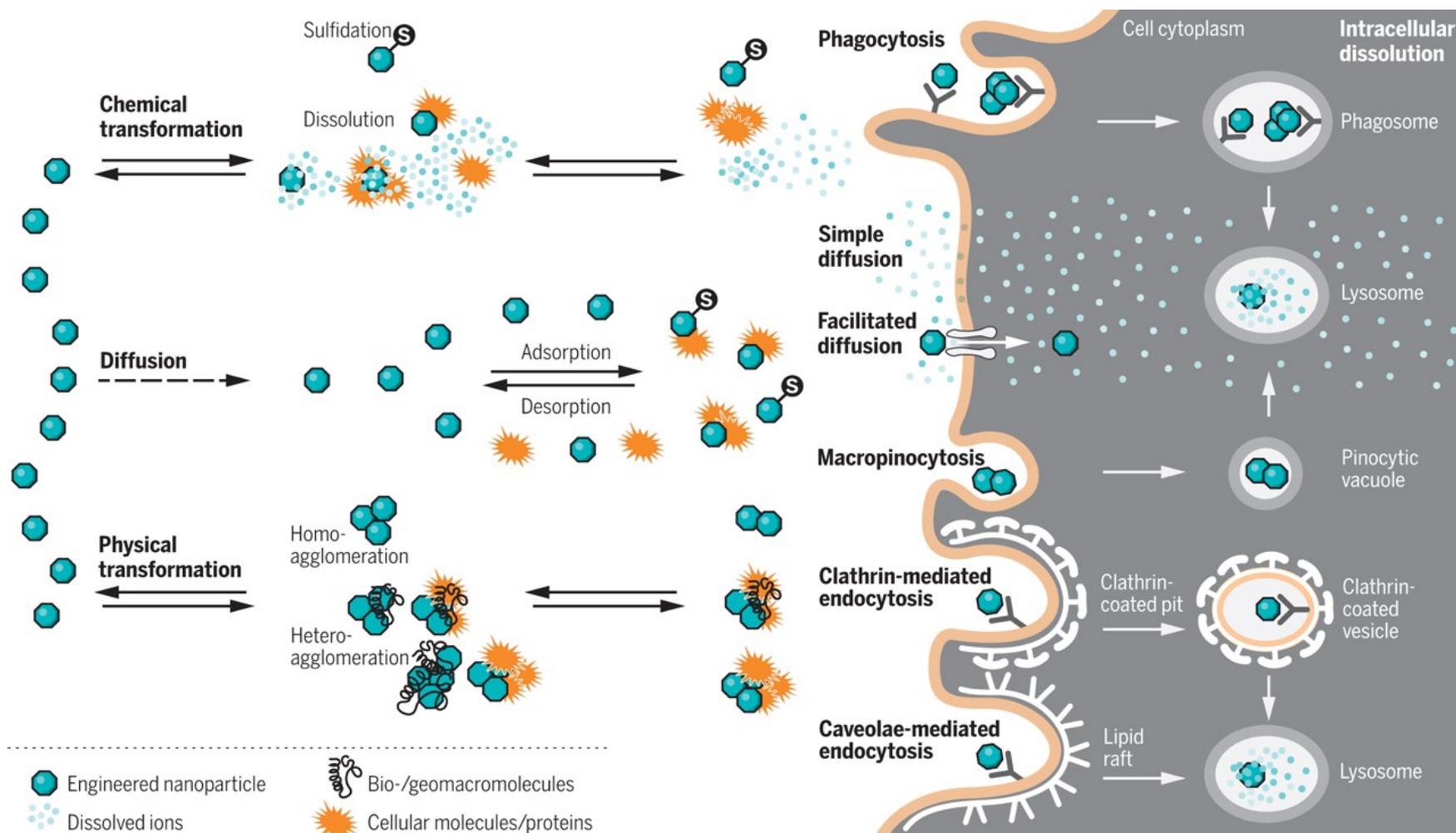
What's special about nanomaterials?

1960s	2007	2017
'Protein adsorption'	**'Protein corona'**	**'Biomolecular corona'**

'Protein adsorption'
- Liposomes **and** polymeric NPs
- *Ex vivo* and *in vivo* investigations
- **Qualitative** characterization
  - Gel electrophoresis
- **Pharmacology** of NPs
  - Functionalization (PEG dilemma)
  - Opsonization
  - Blood circulation half-life

'Protein corona'
- Lipid, carbon, metal-based NPs
- *Ex vivo* investigations
- **Protein** characterization
  - Mass spectrometry
- **Biological impact**
  - Cytotoxicity
  - Cell internalization
  - Targeting

'Biomolecular corona'
- Lipid, carbon, metal-based NPs
- *Ex vivo* and *in vivo* investigations
- **Molecular** characterization
  - Mass spectrometry
  - Genomics
  - Lipidomics
  - Metabolomics
- Biomedical **exploitation**
  - Targeting
  - Diagnosis
  - Drug delivery etc.

https://doi.org/10.1038/nnano.2017.61

Nanomaterials transformation
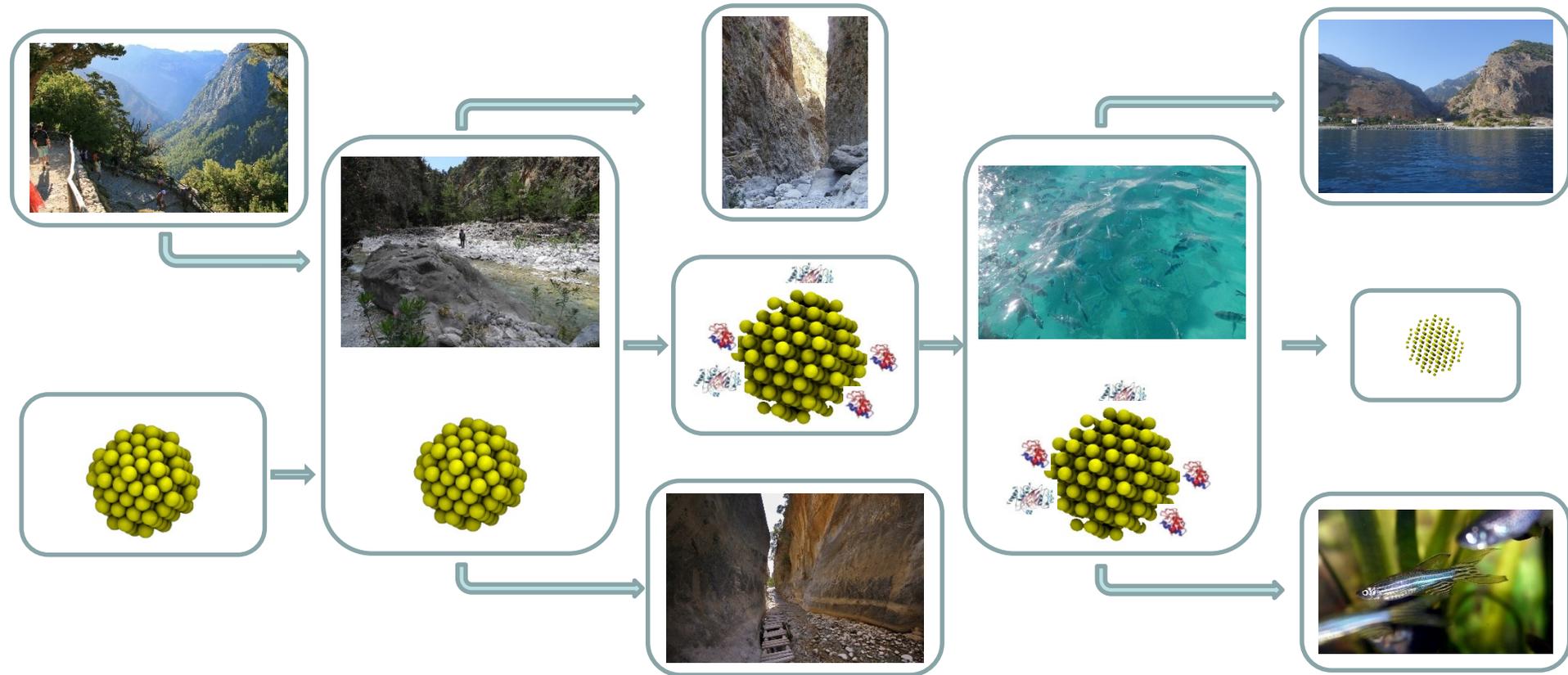
- **A released nanomaterial will change itself and affect its surrounding environment**

Data Curation & NIKC Instance
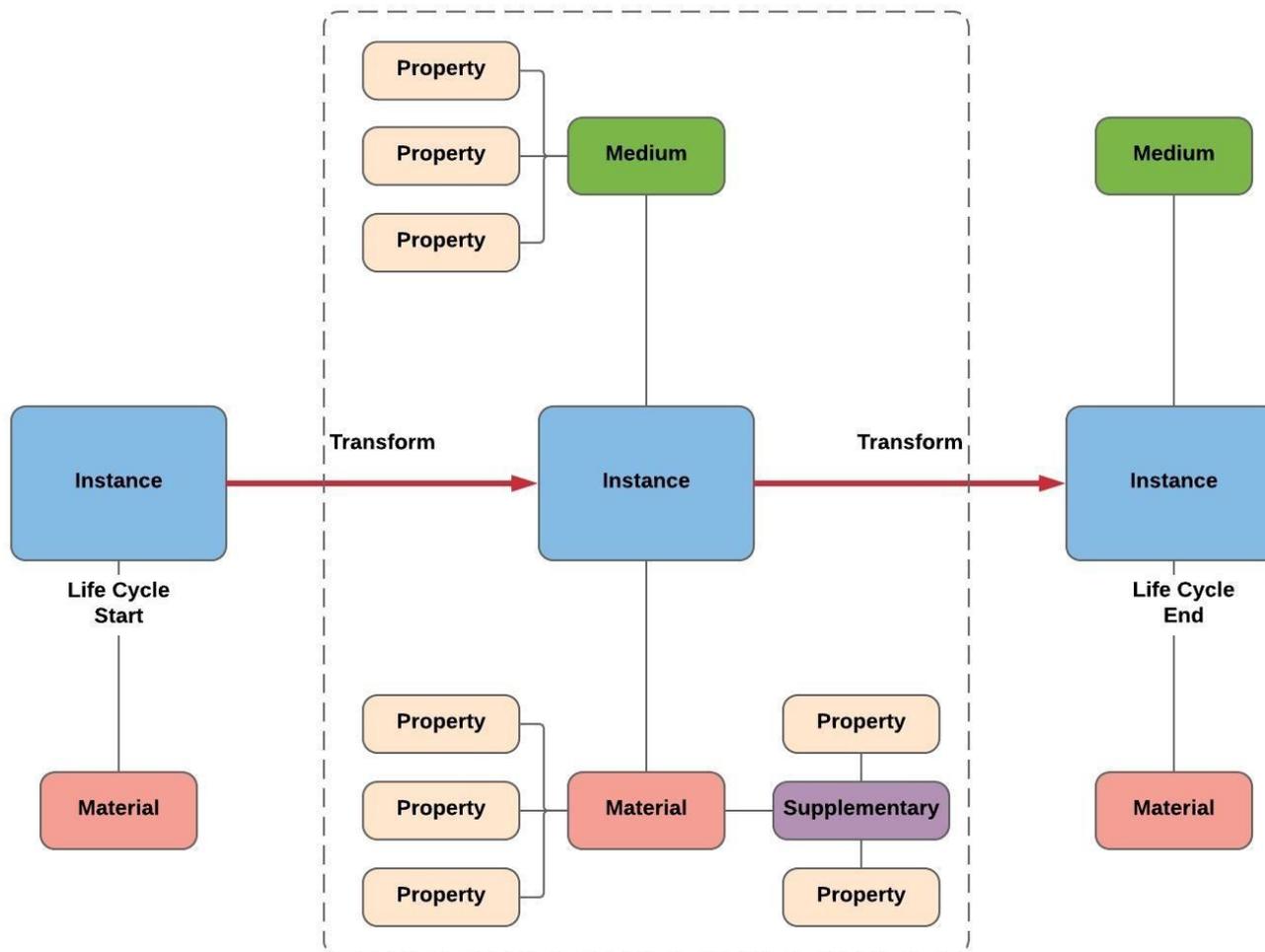
**Data Curation: The process of data collection and organisation**

Building on OpenRiskNet approaches

Service-oriented science

- Standardize
  - Agree on e.g. interfaces, data formats, protocols etc.
- Decompose and compartmentalize
  - Experts (scientists) provides services
  - Achieve interoperability by exposing data and tools as Web services via APIs
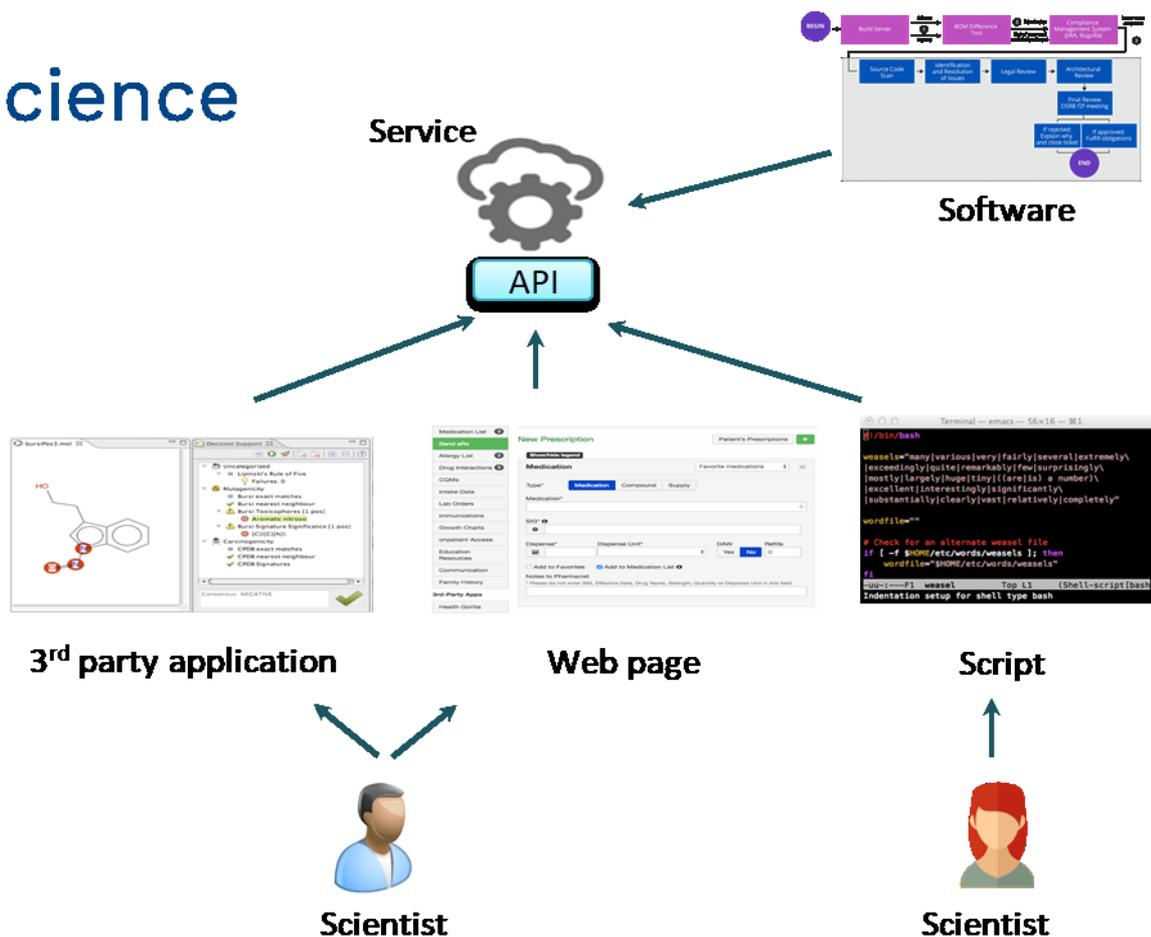
NanoCommons data management tasks
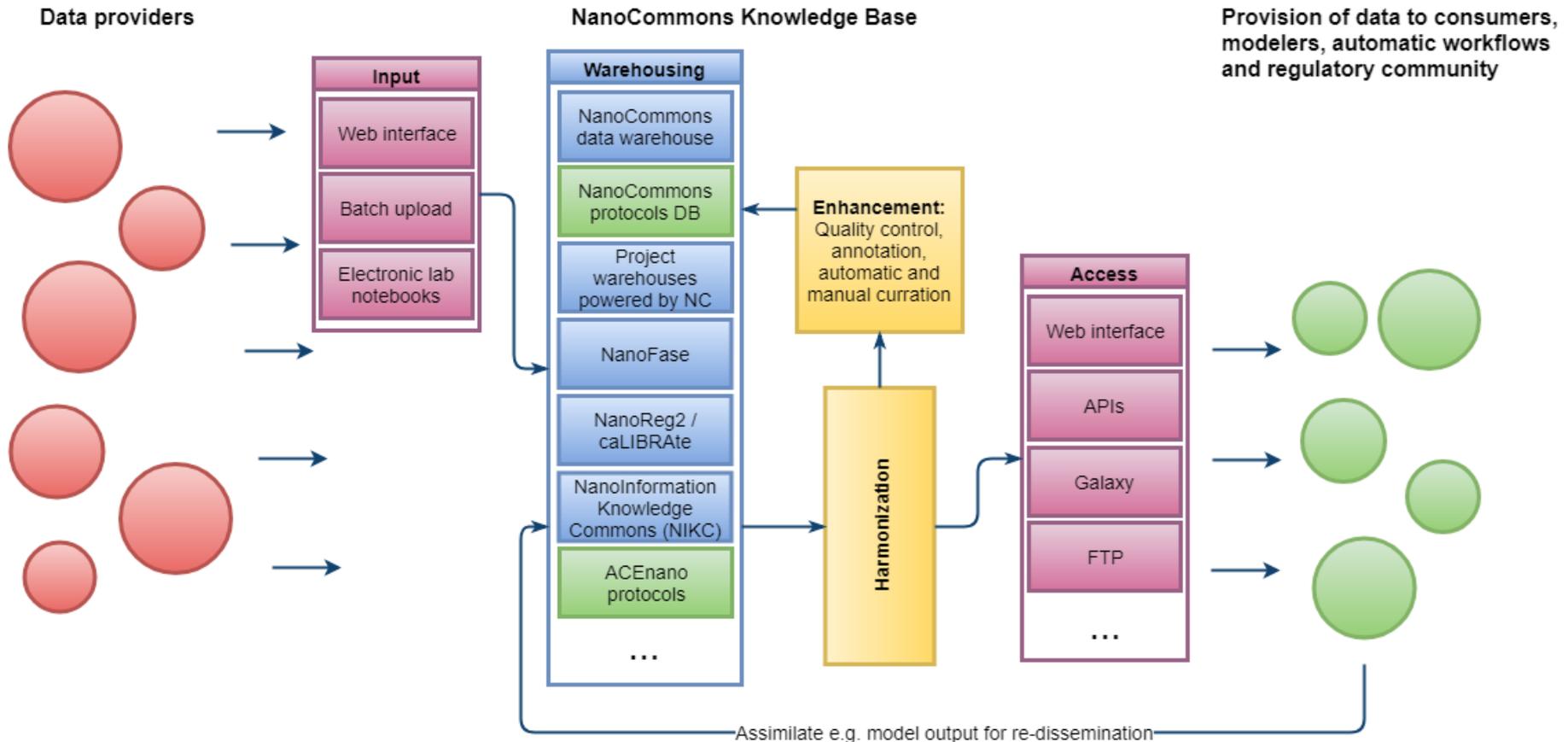
Using multiple APIs – federating databases and semantic mapping layer on top – flexibility for data providers
Using Jupyter notebooks – data pulling, data pushing, modelling, standardised reporting templates etc.

Semantic interoperability
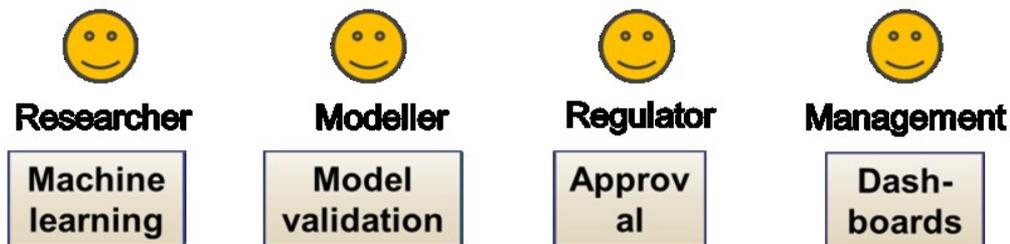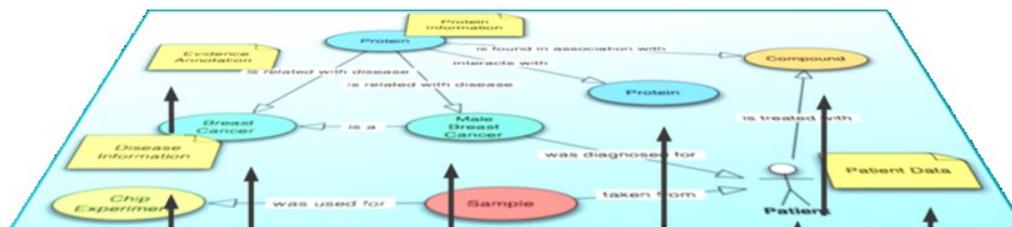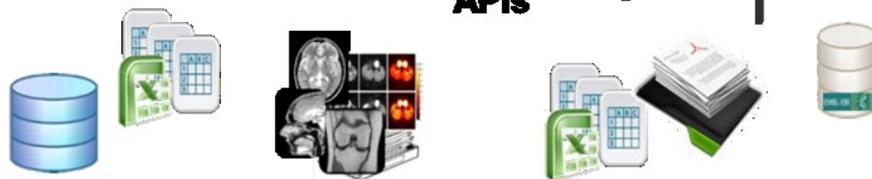
Key lessons from OpenRiskNet

- Data licensing and data ethics statements as condition of (*in vivo*) data integration

- Ethical approval / animal licence etc. as part of the metadata linked to the dataset

- Protocols integrated as data / metadata

Copyright 2009 by Randy Glasbergen.
www.glasbergen.com

"Lately I've been feeling ethical. Can you prescribe something for that"

Service descriptions & discovery

- 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.

- Web: https://infrastructure.nanocommons.eu/

	Date Created
	Date Updated
	Date Published
	Name
	URL
	API URL
	API Type
	Provider name
	Provider contact
	Provider organisation
	Category
	Service type
Service identification	Implementation status
	Technology readiness level
	Licence type
	Licence
	Login required
	Tagline
	Description
	Applicability domain
	Topic
	Biological area
	Targeted industry
	Targeted users
Training and user support	User support service
	User support contact
	Documentation center
	References

Service descriptions and discovery

General description

Direct URLs to the service

Service identification

Training and user support

Contact and additional information on licence, TRLs, etc.

NanoCommons Services

Jaqpot GUI

Generate, store and share predictive statistical and machine learning models

Jaqpot is a user-friendly web-based e-infrastructure containing many data analysis and modelling microservices integrated under harmonised APIs. Jaqpot GUI 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 has been developed by the Unit of Process Control and Infromatics in the School of Chemical Engineering at the National Technical University of Athens.

Go to service →   API definition →

Type: Workflow, Application, Visualisation tool, Analysis tool, Processing tool, Trained model, Model generation tool, Model, Data mining tool
API Type: Based on Jaqpot API that uses REST under OpenAPI2 specification
Categories: Knowledge bases, Processing and analysis, Visualisation and reporting
Applicability domain: Computational modelling, Predictive toxicology
Topic: Predictive modelling
Targeted industry: Chemicals, Nanotechnology
Targeted users: Data managers, Risk assessors, Researchers, Students

Support service: https://github.com/KinkyDesign/jaqpot-web/issues
Documentation: https://github.com/KinkyDesign/jaqpot-web/
References and training materials:
  • Chomenidis et al, 2017 (https://pubs.acs.org/doi/abs/10.1021/acs.jcim.7b00223)
  • Video: https://www.youtube.com/channel/UC-j4T5s5li4iMm75AAOiJ7w

Provided by: National Technical University of Athens
Contact: hsarimv@central.ntua.gr
Licence: GNU Lesser General Public License 3 (LGPLv3.0)
Login required: Yes
Implementation status: Graphical user interface available
Technology readiness level: TRL 7 – system prototype demonstration in operational environment

Services tailored by stakeholder / user

OpenRiskNet
RISK ASSESSMENT E-INFRASTRUCTURE

e-Infrastructure   Resources & Training   Participate   Events   News   About

Resources & Training

This page contains resources and training materials to support OpenRiskNet users in getting familiar with the services and tools available in the e-infrastructure. On top of tutorials and video demonstrations, you will also find information on our publications (e.g. peer-review articles, presentations, posters) that may help you further in learning about OpenRiskNet concepts and implementations.

| Category | Risk assessors | Organisations involved | Filter | Reset |

Identification and Linking of Data related to AOPs of AOP-Wiki [AOPLink]   Report
Marvin Martens and Egon Willighagen (Maastricht University, Department of Bioinformatics - BiGCaT)
7 Oct 2019

↓

The NanoCommons offer

- NanoCommons **integrates the nanomaterials communities** around an agreed set of approaches for **data generation, data management and nanoinformatics** to support the risk and hazard assessment of NEMs.

- NanoCommons is **integrating and developing tools and services** for use by the nanomaterials communities

- These tools and services can be **accessed** through the **NanoCommons Transnational Access scheme**

Experimental Workflows Design & Implementation

Data Processing & Analysis

Data Visualisation & Predictive Toxicity

Data Storage & Online Accessibility

OpenRiskNet case study approach

Key requirements:

- Extensible
- Interoperable
- Scalable

Coherent vision of what each is demonstrating and how they are interlinked and provide a complete computational workflow…..

NanoCommons has some way to go to achieve this level of sophistication…….
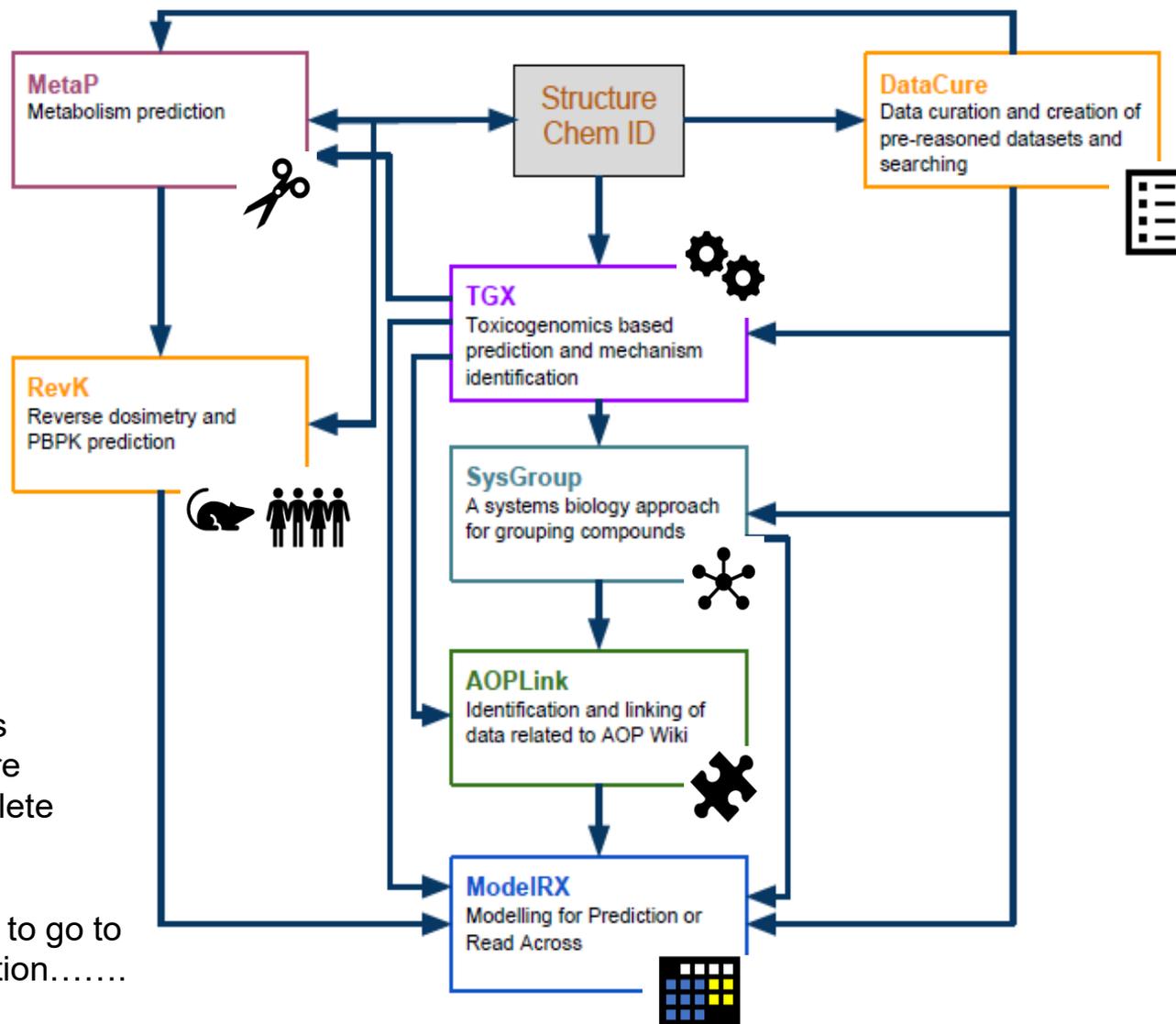
NanoCommons case studies

Dataset curation & integration

Services & Sustainability

Jaqpot models

Enalos tools

NanoPHEAT

Knowledgebase utilisation

NanoCommons Knowledge Infrastructure
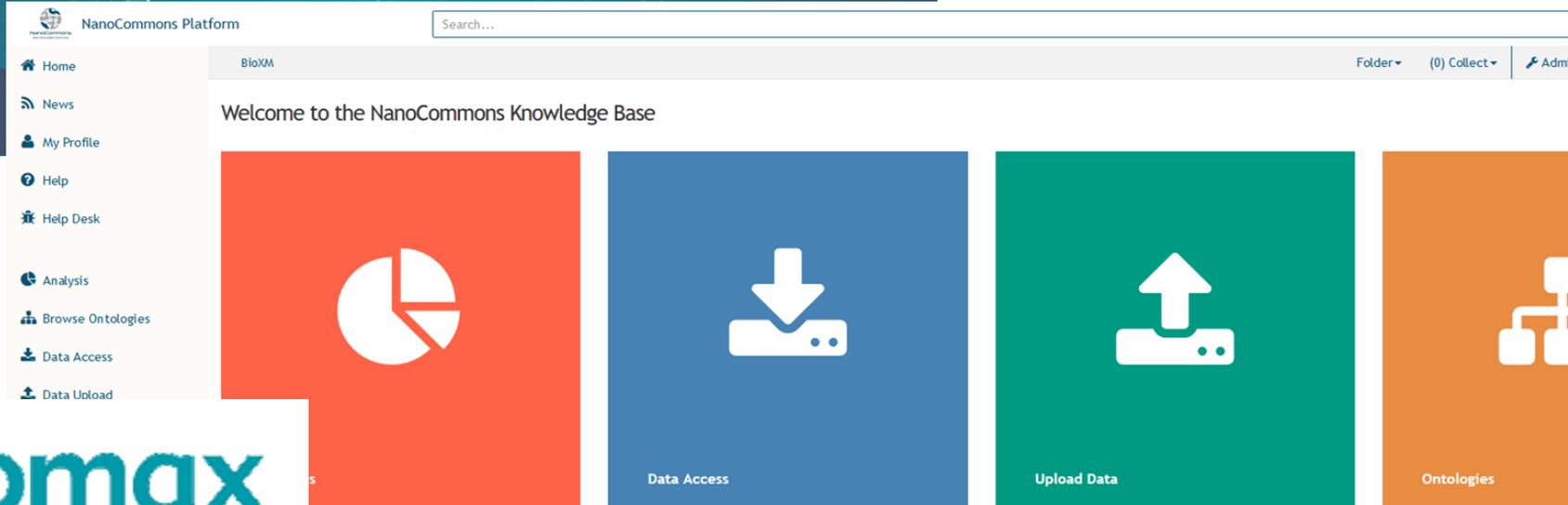
Data management, data lifecycle & metadata

Data warehousing: external data sources

- ## eNanoMapper

- ## NIKC and NanoFase

- ## ACEnano
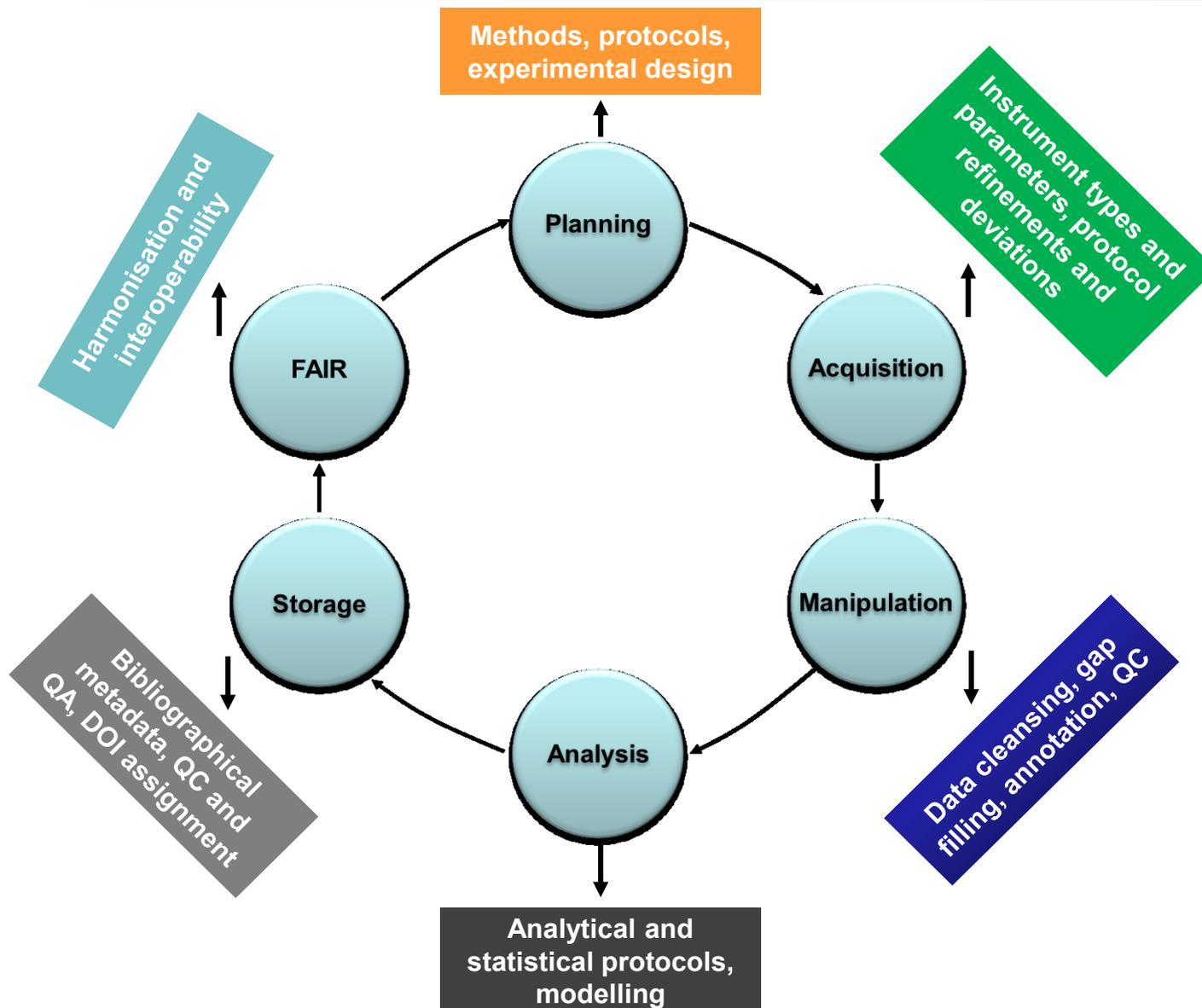
NanoCommons Corona prediction Tool

Nanomaterials image analysis tools


Figure 1: Image upload parameters. [A] Browse button. [B] Nanomaterial type list: Circular/Cylindrical/ Plates/Other.

http://enaloscloud.novamechanics.com/EnalosWebApps/NanoXtract/

Nanomaterials image analysis tools

NANO-IMAGE

Extracting data from microscopy images

LEARN MORE

https://app.jaqpot.org/nanoImage/

Our consortium
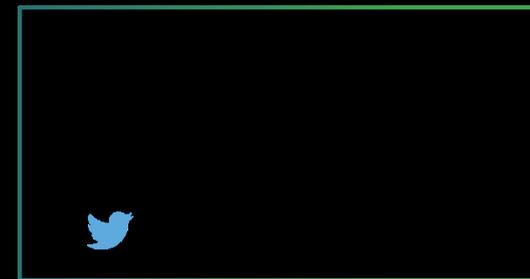
Thank you
for your attention!

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Dieter Maier, Beatrix Gerhard
BioMax Informatics AG

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University of Birmingham

Egon Willighagen, Marvin Martin
Maastricht University