



NanoCommons

Nano-Knowledge Community

Integration of knowledge & services

Thomas Exner (7P9)

SbD Workshop

9th November 2021

How we can work together?

- 1) Knowledge collection and exchange
- 2) Findability of approaches
- 3) Data sharing
- 4) Nanoinformatics tool and platform integration
- 5) Support from TA projects

1) Knowledge exchange

Demonstration cases:

1. Best-practice in study design and its documentation for nanosafety evaluation
2. Best-practice in SOP development for nanosafety assessment
3. Support for project clusters: Safe-by-Design, risk governance, pilot production facilities and innovation hubs
4. Data and informatics tools for use in nanomaterial risk assessment
5. Development of an InChI for nano (NInChI)



1) User guidance (handbook)

NanoMaterialCommons
User Handbook

Q Search NanoMaterialCommons User Handbook

Home

Data management

FAIRification

Nanoinformatics

Training courses

Demonstration cases

About & partner projects

Data and nanoinformatics shepherds' user guidance handbook

This online resource collects and organizes knowledge and training materials for the two strongly interlinked areas of data management for nanomaterials and nanoinformatics.

If you are a

- scientist (wet or dry lab), who produces and wants to share data
- data manager, curator or steward and want to become more
- computer geek

in the area of nanosafety, nanoinformatics or material safe-by design or want to become one, then this handbook is for you.



<https://nanocommons.github.io/user-handbook/>

Data
management

FAIRification

Nano-
informatics

1) User guidance (handbook)

Data management: general and specific aspects






The data management life cycle

Based on: Papadiamantis, et al., 2020




Despite its significance, structured (meta)data capturing and management (by yourself, your team or the public) is not widely implemented in view of the general perception of data management as being something that is done at the end of a study / project and after the data are fully analysed and processed. This is not the case as accessing original data files or extracting data from a publication requires the necessary metadata. It is needed to shift the design and implementation of data management to the project outset. It is imperative to encourage (meta)data upload to data management systems, to protect intellectual properties where necessary, and with automation. As a result of the cyclical nature of the data lifecycle, it is always possible to improve coverage, taking into account the needs of different users and requirements.



The resources below will give guidance how such a distributed (meta)data collection and management can be organised for the nanosafety and nanoinformatic areas:

-  [Roles and responsibilities](#) →
-  [Data completeness, minimum information checklist, data quality](#) →
-  [Electronic lab notebooks](#) →
-  [Nanosafety data resources](#) →
-  [NanoCommons data workflows](#) →

And some big resources on data management more generally and neighbouring areas:

-  [Open Science Training Handbook](#) →
-  [Chatham House Guide: Principles for Sharing the Data and Benefits of Public Health Surveillance](#) →
-  [Chatham House Resource](#) →

1) 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.

The NanoMaterialCommons User Handbook is © 2020-2021 and distributed by Creative Commons Attribution 4.0 International License.

[Edit this page on GitHub.](#)



Q Search NanoMaterialCommons User Handbook

Data management

NanoCommons
Data Warehouse

NanoCommons
different e
publicly re

To be able to

- 1 NanoCommons
NanoCommons
interfaces
- 2 NanoCommons
made pub

For the data
and browsed
data provider
they want to
NanoCommons

Access

 NanoCommons

Training

The session fr
how to use th
Background o
governance f
it covers the
does or is res
formation ar
the protein co
Herein you ca
parameters th
You also find
can start ther



Q Search NanoMaterialCommons User Handbook

Data management / Nanosafety data resources / ACEnano Knowledge Infrastructure

ACEnano 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.

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.



 ACEnano Knowledge Warehouse manual →

 Slides from the NSC Week 2019 - Introduction →

 Slides from the NSC Week 2019 - Training →

2) Service listing



Services

Library

Events

About

Data Visualisation & F ▾

Service type ▾

Regulators ▾

Filter

Reset

Submit a service

NanoCommons Knowledge Base access within KNIME through Enalos APIs

Enalos APIs, KNIME, NanoCommons Knowledgebase

This KNIME nodes give access to the NanoCommons Knowledgebase-annotated nanomaterials datasets through Enalos APIs. Physicochemical, toxicological and omics characterisation data such as DLS, Zeta potential, TEM size, % of viable ...

Provided by: NovaMechanic Ltd

Type: Data curation tool, Modelling tool, Data warehouse, Knowledge base
Applicability domain: Hazard assessment, Risk assessment, Risk characterisation, Bioinformatics, Exposure assessment, Nanoinformatics, Safe by design

Guidenano Tool

The European Union FP-7 project GUIDEnano has developed a web-based guidance tool for users to apply the most appropriate risk assessment and mitigation strategy for NM-enabled products throughout their life ...

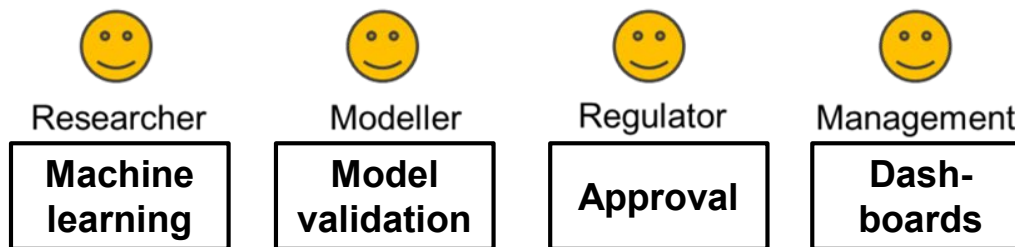
Provided by: LEITAT Technological Center

Type: Modelling tool

Applicability domain: Hazard assessment, Risk assessment, Risk characterisation, Exposure assessment

Topic: Information extraction, Kinetics / biokinetics, Predictive modelling, Toxicology, Ecotoxicology

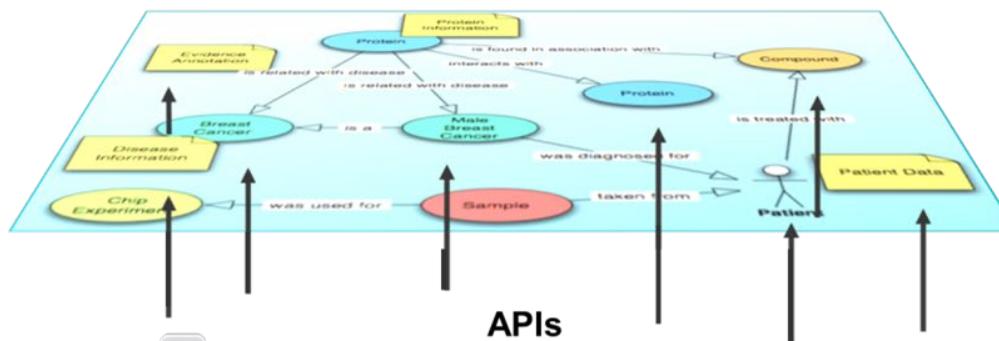
3) Data sharing



UI ↑ API

Query & analyse based on semantic model

Semantic Model



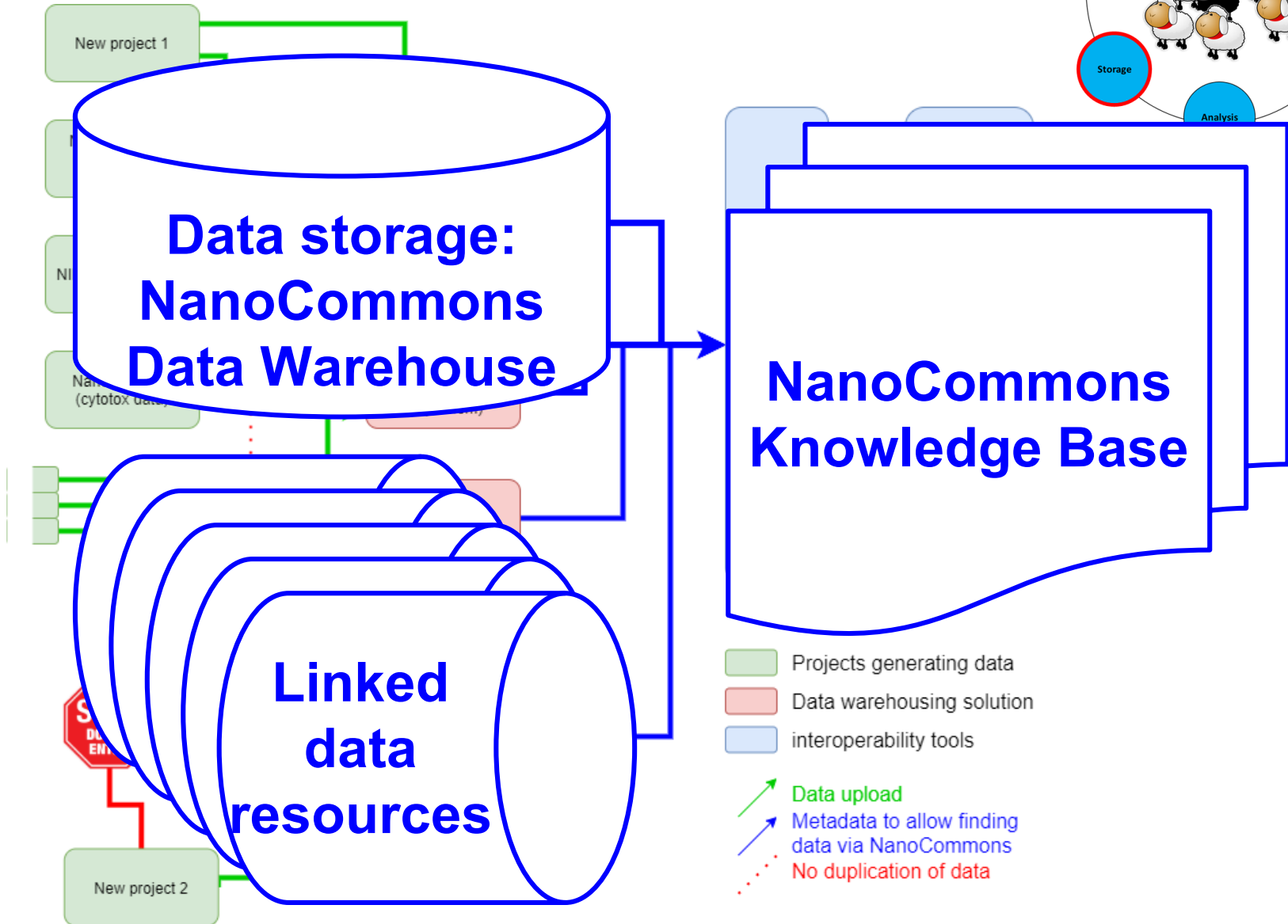
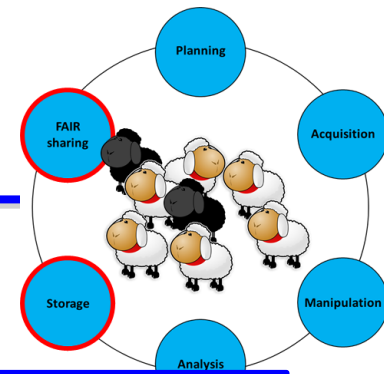
Semantic integration of different data types

Original DBs



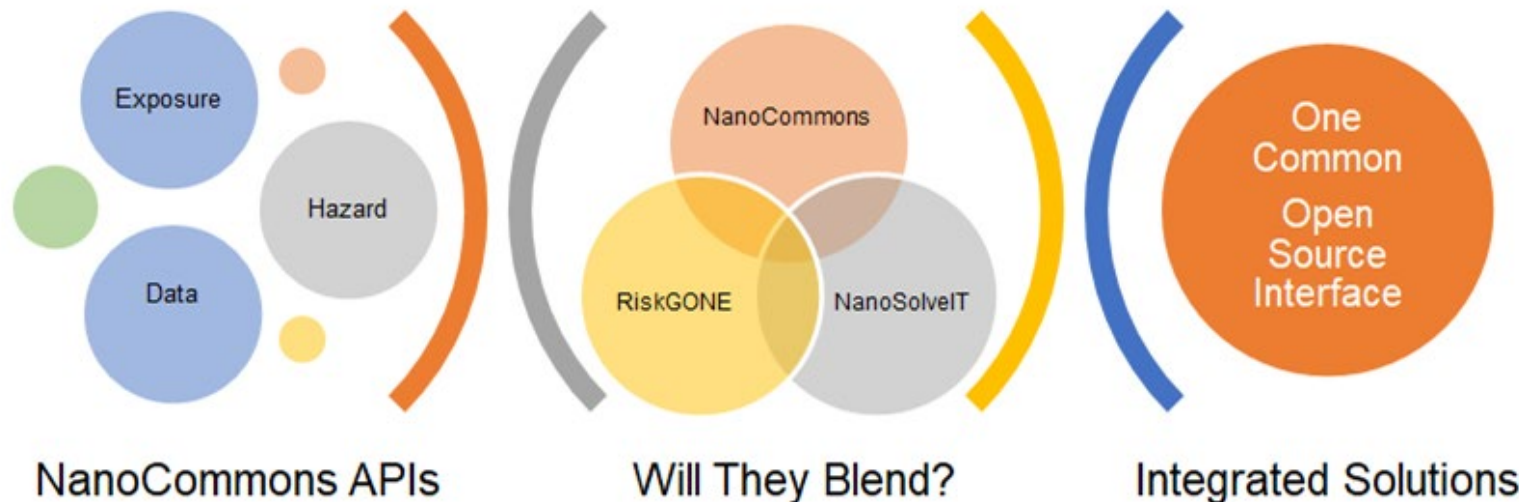
NanoMILE/NanoFASE/NanoReg/eNanoMapper

3) Data sharing





4) Combining nanoinformatics platforms



The screenshot shows the Jagpot web interface. The top navigation bar includes the Jagpot logo, a search bar with the text 'model', and user profile icons. The main content area displays a list of models under the heading 'Models > Shared > With NanoCommons'. The list includes:

- Model title: PBPK model for 99m-Technetium-labelled carbon nanoparticles (Nov 8, 2021)
- Model title: Naive Human PAA-PEG PBPK Model (Oct 7, 2021)
- Model title: Bayesian Network for predicting nanomaterial hazard v1 (Sep 28, 2021)
- Model title: PAMPA MODEL (Sep 13, 2021)
- Model title: Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents (Mar 31, 2021)
- Model title: Linear Model for Predicting Solubility of C60 Fullerenes in Various Solvents (Mar 26, 2021)
- Model title: Naive Bayes model for the prediction of cytotoxicity of metal oxide nanoparticles (Nov 15, 2020)
- Model title: Stochastic TiO2 inhalation PBPK model on mice (Jul 7, 2020)

A detailed view of the 'PBPK model for 99m-Technetium-labelled carbon nanoparticles' is shown on the right side of the screen. The details include:

- Model**
- Owner:** Periklis Tsiros
- Created:** Nov 8, 2021
- Description:** Web implementation of the PBPK model presented in Pery et al. (2009)

5) Support

NanoCommons TA quick-guide

This NanoCommons quick-guide offers an overview of the steps required to apply for the NanoCommons TA, along with a detailed. While Users can follow this guide to apply, it is strongly recommended to go through our [detailed guidelines](#) to ensure alignment with all necessary requirements.

Applying for access

1. **Who can apply:** No fee open access is available for Transnational Access for Users from industry, regulators or research institutions located in EU member states and associated states. EC financial support requires that the results of the work carried out are intended for publication. For more details see section 2.7.2 Conditions of access of the [NanoCommons User Guidelines](#).
2. **What does the award cover:** The award covers all research costs in the form of a daily rate. This will be calculated directly from your application form and therefore you need to have discussed your project with your proposed host technology expert in advance of submission. You will not be required to formulate a budget.
3. **Application:** You can apply for access for NanoCommons TA at any time during an open call via the online application form (<https://www.nanocommons.eu/apply-for-access>), and all applications will be reviewed together about 4-8 weeks from the call closing date.
4. **Before you apply:** Define the work you would like to carry out, ensure that it is covered from the offered NanoCommons offered services (<https://www.nanocommons.eu/e-infrastructure/transnational-access-services/>) and discuss your ideas directly with the technology expert at the appropriate TA partner or contact the NanoCommons Helpdesk (<https://www.nanocommons.eu/helpdesk>), who will direct your query to the relevant TA partner and technology expert.

Online application

1. **Registration:** To apply you need to register at <https://www.nanocommons.eu/apply-for-access> and fill in the online application form.
2. **Applying:** Should a User apply for access to services from more than one TA partner in the same project application (joint application) a clear justification is required. For a joint application the User must submit one application indicating on the application form that it is a joint application and indicating the two or more TA partners that the User needs to access. All applications need to be submitted before the designated deadline for them to be eligible for consideration.
3. **Personal details:** The application form has two sections. Firstly, the Personal Details section which ensures that you do not have to re-enter your personal information for each subsequent TA application. This information will be attached to each TA application upon submission. If you wish to update these details please go into the 'Update your details' section to amend and save them. Any personal information submitted to NanoCommons will be treated according to the GDPR requirements of the



NanoCommons

Nano-Knowledge Community

Thank you!

***Please remember / post your questions
for the final discussion***