



**NanoCommons**

Nano-Knowledge Community

# **The vision: an e-infrastructure combining SbD platforms**

*Iseult Lynch (UoB) & Thomas Exner (7P9)*

*SbD Workshop  
9th November 2021*

# Positioning of NanoCommons (2018-2021)



**JRC** **OECD**  
EUROPEAN COMMISSION  
Nanomaterials Sponsorship Programme



NanoSafety Cluster



us-eu  
bridging nanoEHS research efforts



OECD  
Working Party on Manufactured Nanomaterials

Data Integration / Networking



Tools & data input & output



NanoCommons

Knowledge output



EUNCL  
Nanomedicine Characterisation Laboratory

Harmonisation  
Meta-analysis  
Integration across domains  
Federate access to data



EUON  
EUROPEAN UNION OBSERVATORY FOR NANOMATERIALS

Governance projects:



RISK GONE NANORIGO Gov4Nano  
meeting the needs of nanotechnology



ACEnano NanoFASE SmartNanoTox NanoMILE NANO SOLUTIONS GUIDE nano NanoDenine



OpenTox elixir  
Research Infrastructure  
NFFA, EUDAT, CERIC

Safe-by-Design projects:



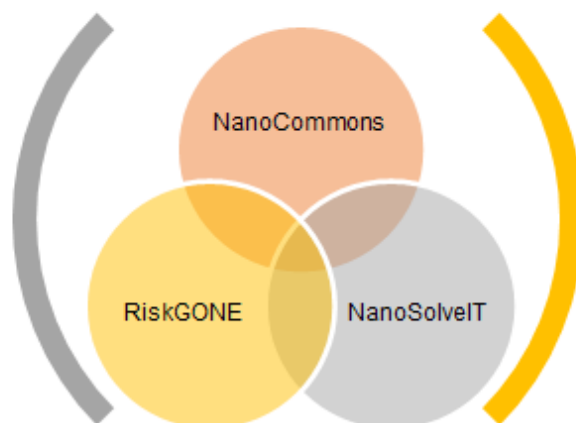
SABYNA SbD Nano ASINA SABYDOMA  
H2020 Safe-by-Design

# Interoperability and Integration

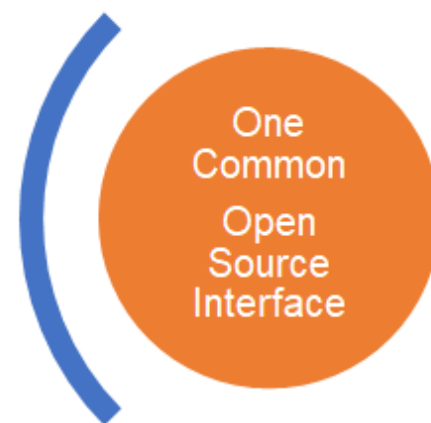
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NanoCommons APIs



Will They Blend?



Integrated Solutions

## Key messages from workshop:

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Why is what NanoCommons does here different?

- Focus on service providers and technical solutions
- Hands-on activities / support
- Support in the form of TA projects
- Open to everyone and across project boundaries
- Focus on sustainable solutions for ALL  
(Containerisation, APIs, KNIME node development etc.)

Ongoing “support” activities:

- NSC working groups (e.g. WG-A, WG-F)
- Governance council (e.g. data core group)
- SbD cluster activities - **this event** - want to do more!

# Integration of tools - output from 1 as input to next...



## Short description

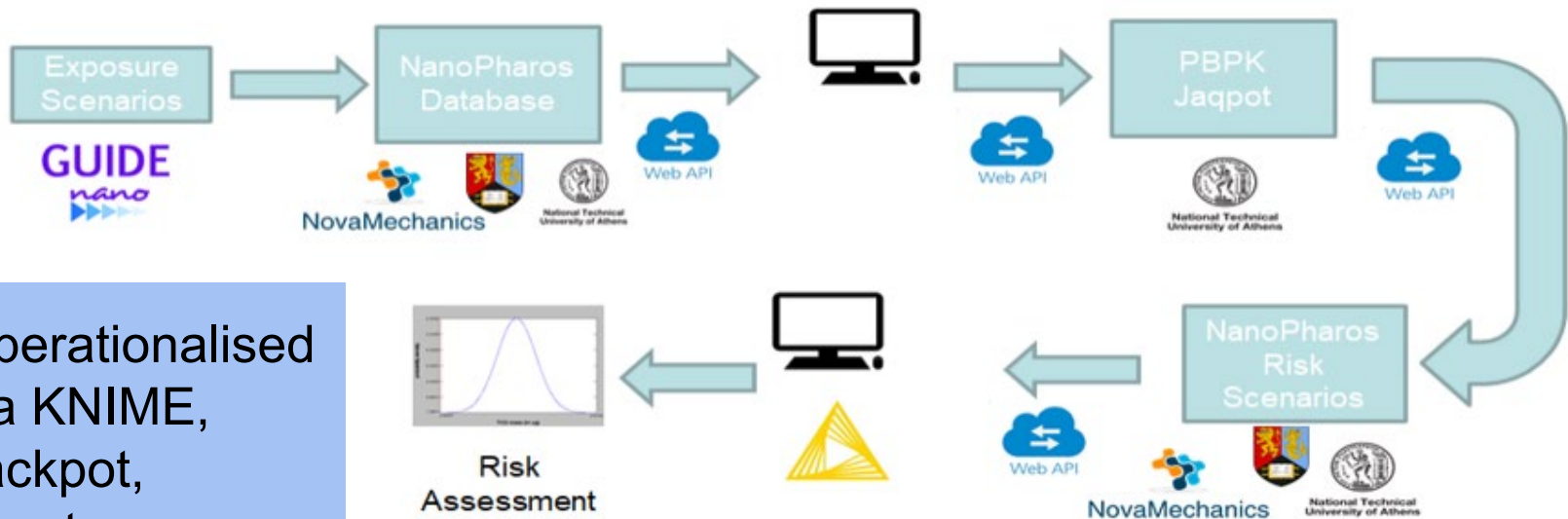
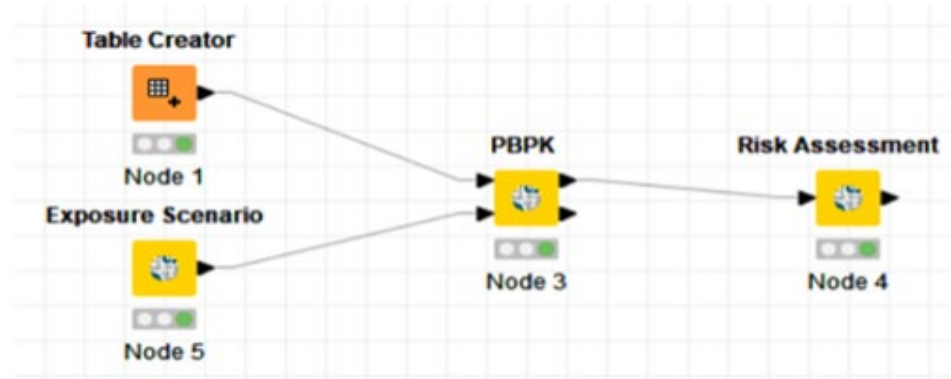
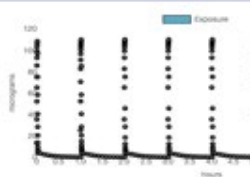
The workflow is a combination of nanoinformatics tools available through the NanoCommons computational infrastructure. This web application, hosted and implemented within [Enalos Cloud Platform](#), estimates the risk of triggering ADP 173 (Lung Fibrosis) in mice due to exposure to 20nm TiO2 engineered nanoparticles.

**External exposure:** Four different exposure scenarios have been simulated using the GUIDENano tool. The user can alternatively enter a custom-made scenario.

### Case 1

45 g (initial mass 3000 kg) of TiO<sub>2</sub> (22nm) poured over 7 hours in the NF, with 1 min activity duration every hour. For every hour the mouse stays 90 s in the NF and spends the rest of the time in the FF.

[Download timeseries](#)



Operationalised via KNIME, Jackpot, Jupetyr notebooks etc.

<http://enaloscloud.novamechanics.com/nanocommons/exposure>

# TA application

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## Specific (tailored) support for individual groups and projects

The NanoCommons e-infrastructure aims to integrate and further develop existing state-of-the-art tools and to develop those that are needed to fill in the experimental, computational and beyond needs of the nanosafety community. The services are covering several areas, like data storage and online accessibility, data visualisation and predictive toxicity, data processing and analysis or experimental workflow design & implementation.



Experimental  
Workflows Design &  
Implementation



Data Processing &  
Analysis



Data Visualisation &  
Predictive Toxicity



Data Storage &  
Online Accessibility

## Demonstration cases

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Collaborative research coordinated by NanoCommons but open to everybody

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)



# TA offer

NanoCommons Transnational Access (TA) provides **access** to

- **Experts** and their knowledge
- State of the art **nanoinformatics and data management tools and modelling and risk assessment services**, and the expertise to implement them successfully.



Experimental Workflows  
Design & Implementation



Data Processing  
& Analysis



Data Visualisation  
& Predictive Toxicity



Data Storage  
& Online Accessibility

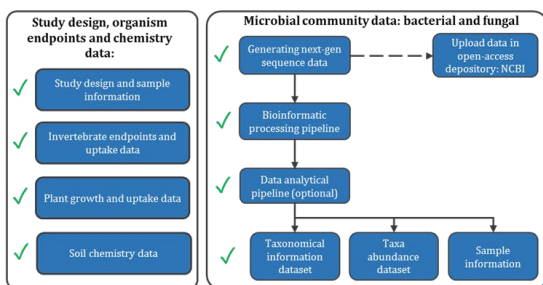


# Experimental workflows



## Experimental Workflows Design & Implementation

### Experimental design / SOP development



API

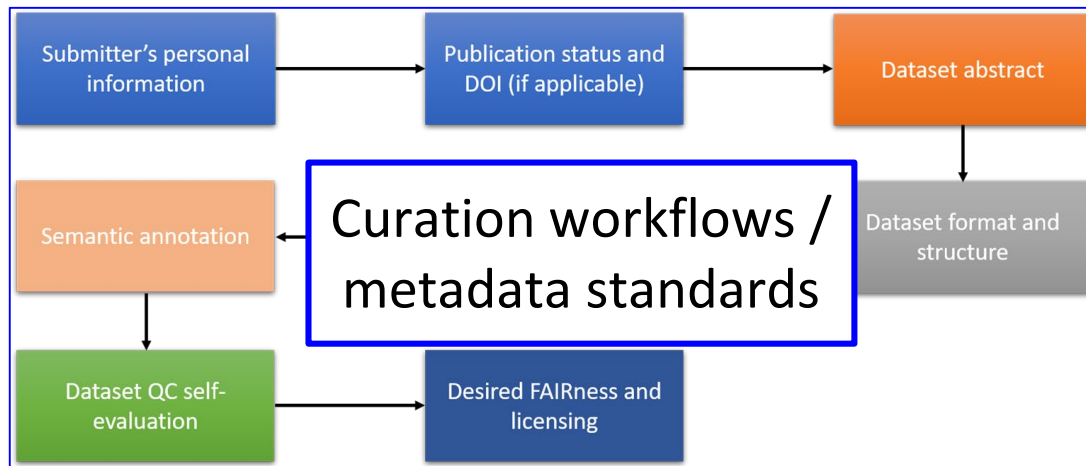
In progress

Integration of datasets and streamlining of informatics pipelines to ensure:

- Transparency
- Accessibility
- Reproducibility



The NIKC Excel Template consists of eight spreadsheet tabs, which are color coded by category: Reference information (3), Experimental results (2), Methods (2), Dictionary (1).



### UoB UV-Vis Round Robin

PROTOCOLS RESULTS ACTIVITY INVENTORIES ARCHIVED RESULTS

Start date: 06/14/2018 15:56 Due date: 08/03/2018 11:41 Status: Task completed (09/04/2018)

Tags: No tags

This SOP describes a sample preparation procedure for particle size measurement of the extinction of light that is measured from the nanoscale. UV-Vis is therefore an ideal technique for the size characterisation of NP suspensions through absorbance at an appropriate wavelength. The results during the subsequent runs.

Ultra-violet Visible Light Spectroscopy (UV-Vis) - SOP v. 2.1

### Electronic lab notebooks

### Protocol steps

1. Materials and Methods | Published on 07/13/2018 12:51 by NanoCommons

#### 1.1 Essential equipment

- UV-Vis Spectrophotometer.
- Calibrated Volume Pipettors of 1 and 5 mL with disposable tips.
- Disposable 3mL cuvettes (Suggested: polystyrene 10 x 10 x 45mm, SARSTEDT, Catalogue number: 67.742).

#### 1.2 Chemicals

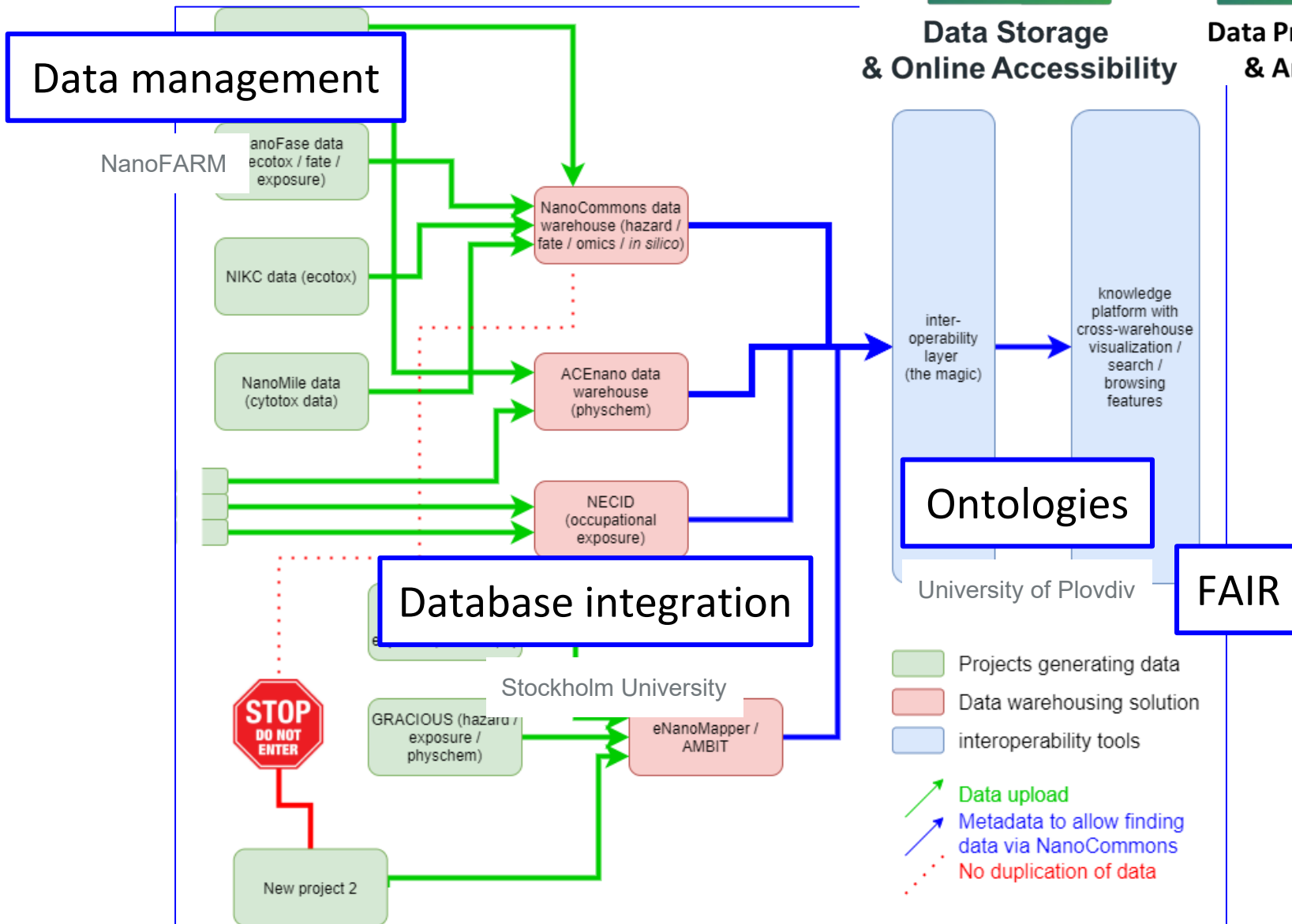
# Data sharing



Data Storage  
& Online Accessibility



Data Processing  
& Analysis



# Analysis and prediction

- nanoQSAR
- Corona modelling
- Image analysis
- Jaqpot/Enalos as modelling platform
- Jaqpot/Enalos as modelling repository
- Integration of tools
- Curation/storage of experimental & computational data

University of Burgos  
(descriptor prediction +  
image analysis)

University of Piemonte Orientale  
(Mesothelioma Expression Profiling)

University of Nevada  
(PBPK)



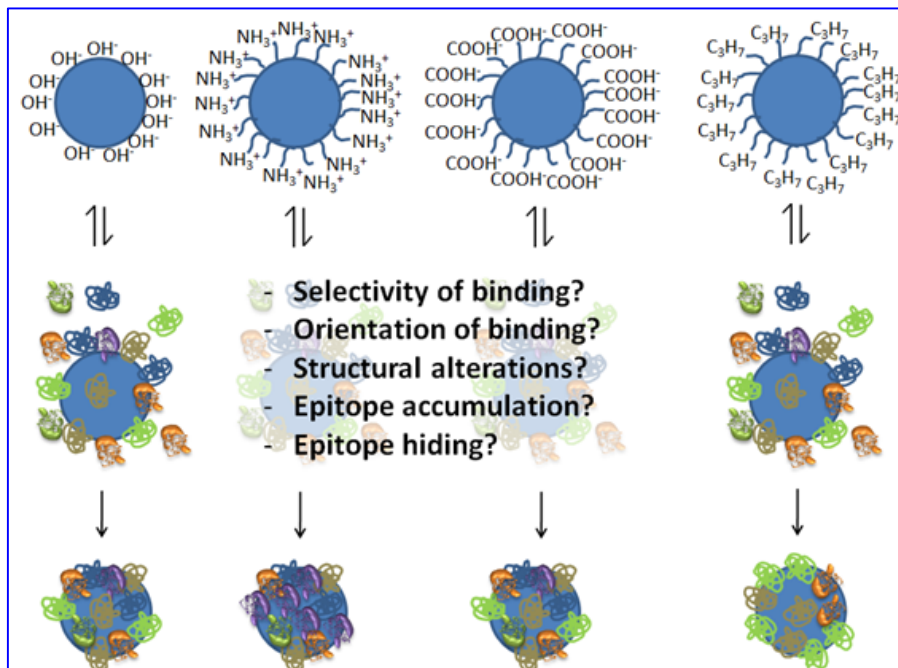
Data Processing  
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Data Visualisation  
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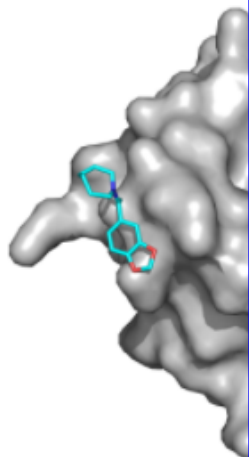
# TA: Diamond SARS-CoV-2 Mpro fragment screening program

## XChem fragment screen

The initial screen encompassed multiple fragment libraries: the [DSI-poised library](#), [MiniFragments](#) (Astex) [FragLites](#) & [Peplites](#) ([CRUK Newcastle Drug Discovery Unit \(Newcastle University\)](#)), [York3D](#) (University of York), [SpotFinder](#) and [heterocyclic electrophilic fragment library](#) (Hungarian Academy of Sciences) and an [electrophilic fragment library](#) designed and pre-screened by mass spec at the Weizmann Institute (see below).

There were 74 hits of high interest views [here](#):

- 23 non-covalent hits in the active site
- 48 covalent hits in the active site
- 3 hits in the dimer interface



## COVID-19 ADMET DATA ANALYSIS

### ADME/PK-traffic lights according to PROSILICO

Traffic lights for optimal oral bioavailability (F), half-life ( $t_{1/2}$ ), once daily dosing and dissolution potential (fdiss)

#### For 3 essential parameters

	Poor	Good	Excellent	
F	<0.4	0.4-0.7	>0.7	>0.85
$t_{1/2}$ (h)	<3; >48	3-8; 24-48	8-24	
fdiss	<0.7	0.7-0.85	>0.85	>0.95

#### For iv dosing (once daily)

Poor	$t_{1/2}$ <3; >48 h
Good	$t_{1/2}$ 8-24 h
Excellent	$t_{1/2}$ 3-8; 24-48 h

#### For oral dosing (once daily)

Poor	If F <0.4 or $t_{1/2}$ <3; >48 h or fdiss <0.7
Good	If F >0.7 and $t_{1/2}$ 8-24 h and fdiss >0.85
Excellent	If Any other result



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*Thank you!*

***Please remember / post your questions***