NanoCommons

Nano-Knowledge Community

The vision: an e-infrastructure combining SbD platforms

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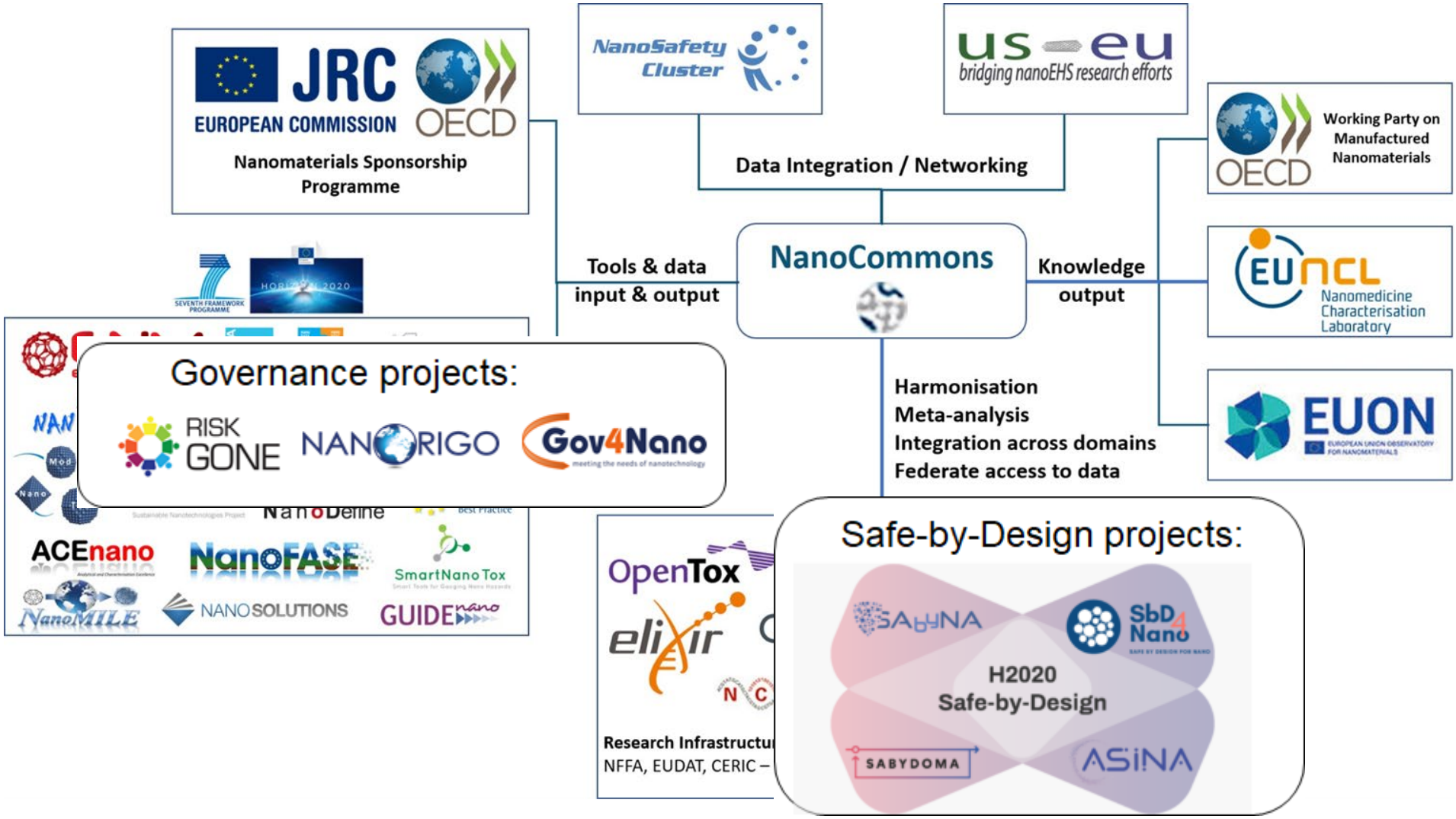
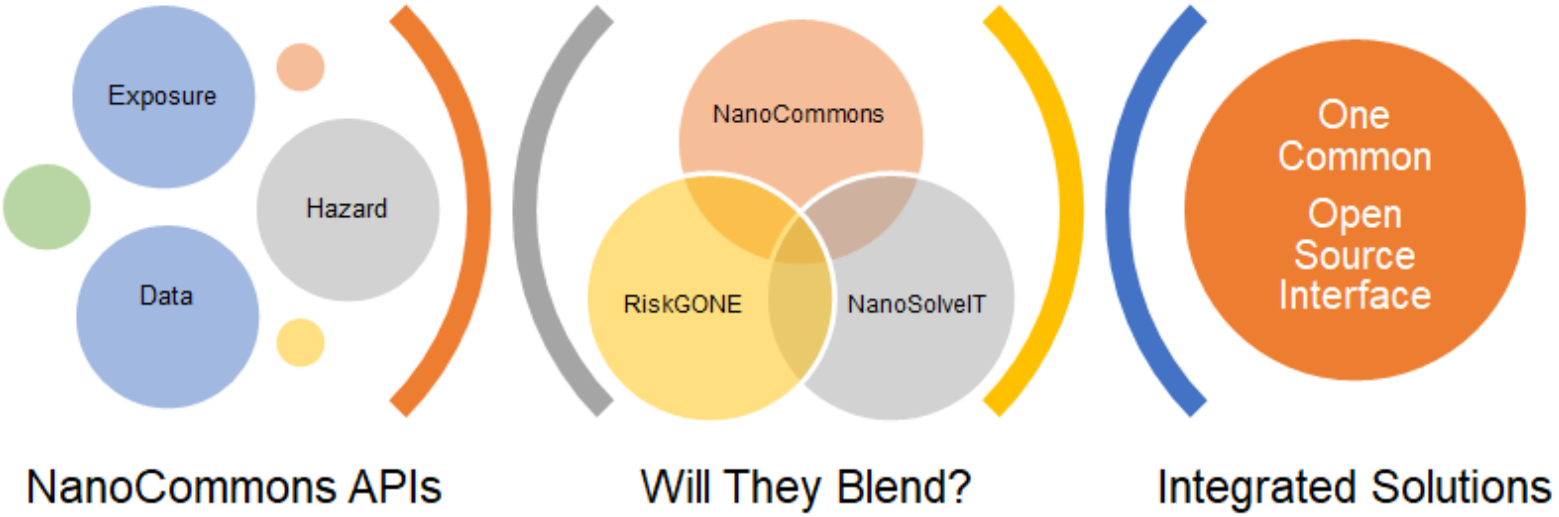
SbD Workshop

9th November 2021

Positioning of NanoCommons (2018-2021)



Interoperability and Integration



Key messages from workshop:

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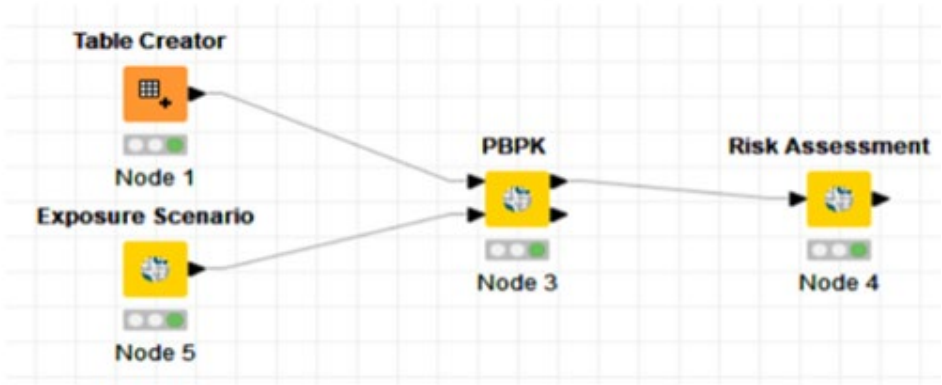
Why is what NanoCommons does here different?

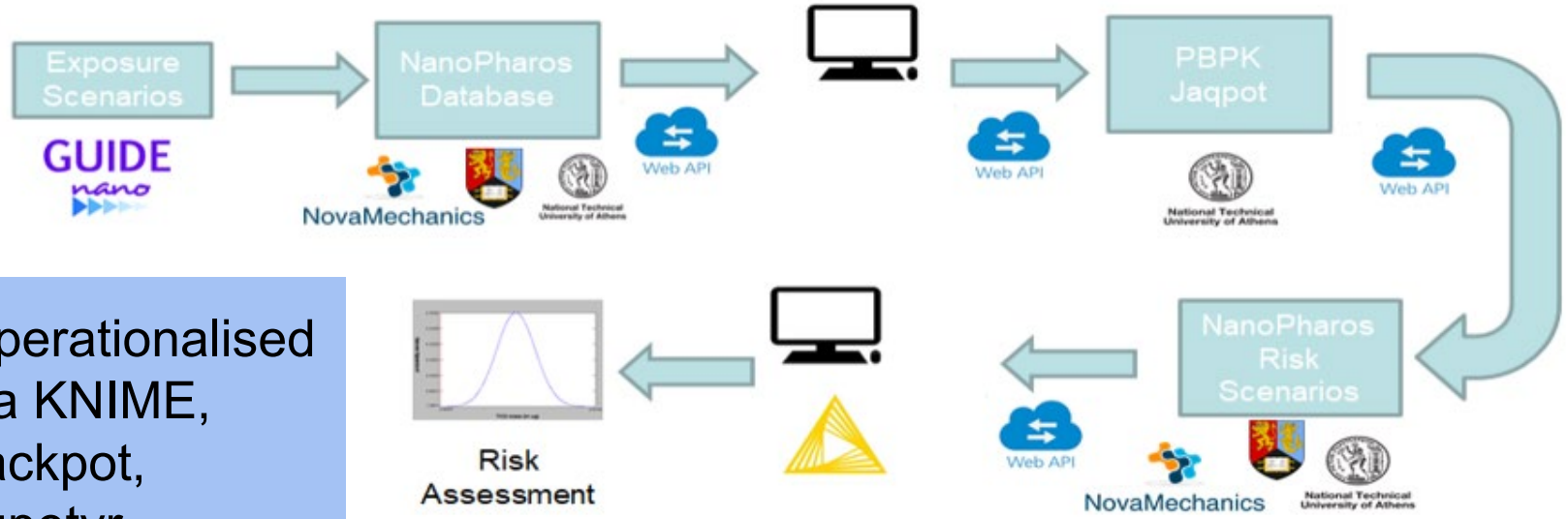
- Focus on service providers and technical solutions
- Hands-on activities / support
- Support in the form of TA projects
- Open to everyone and across project boundaries
- Focus on sustainable solutions for ALL (Containerisation, APIs, KNIME node development etc.)

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…





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

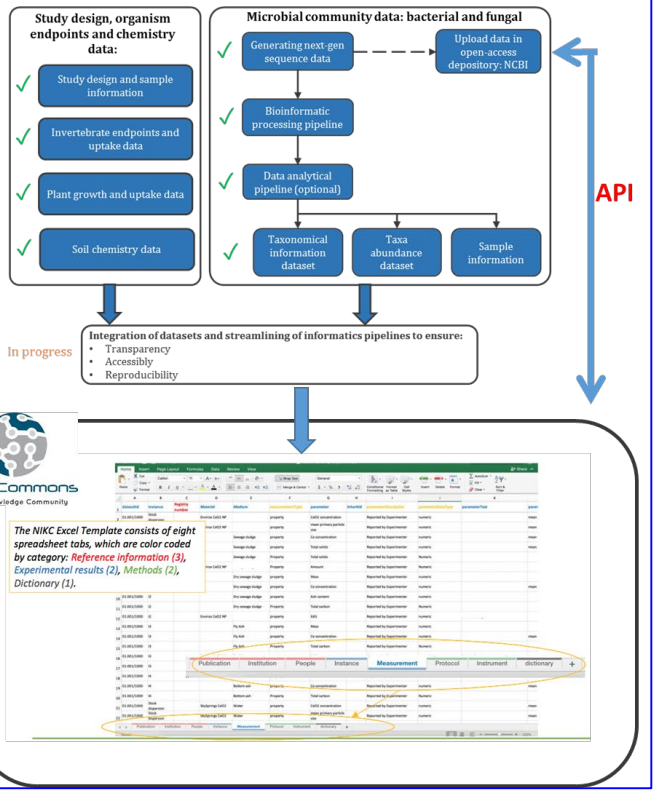
Data Visualisation
& Predictive Toxicity

Data Storage
& Online Accessibility

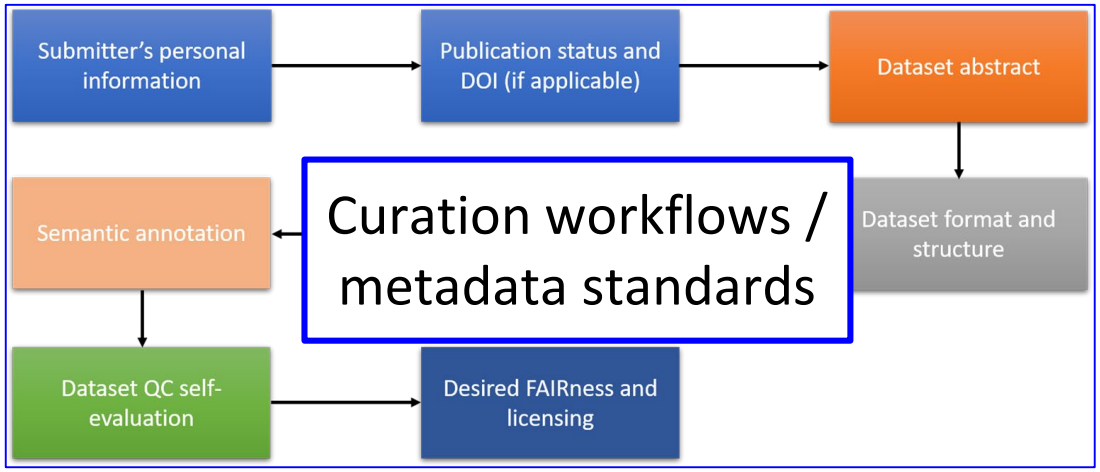
Experimental workflows

Experimental Workflows
Design & Implementation

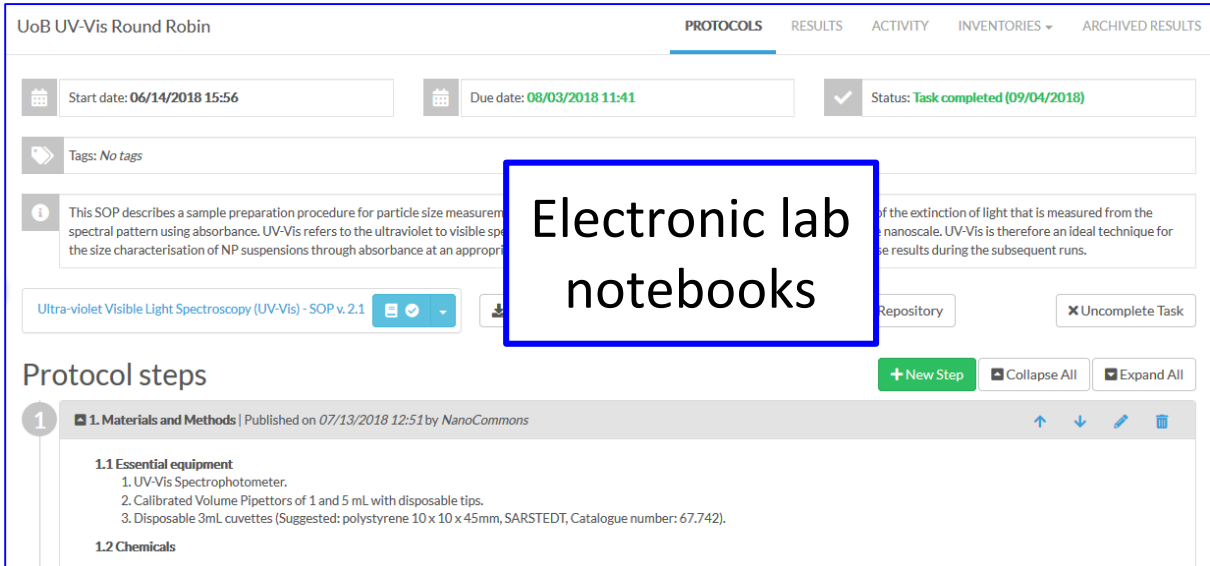
Experimental design / SOP development



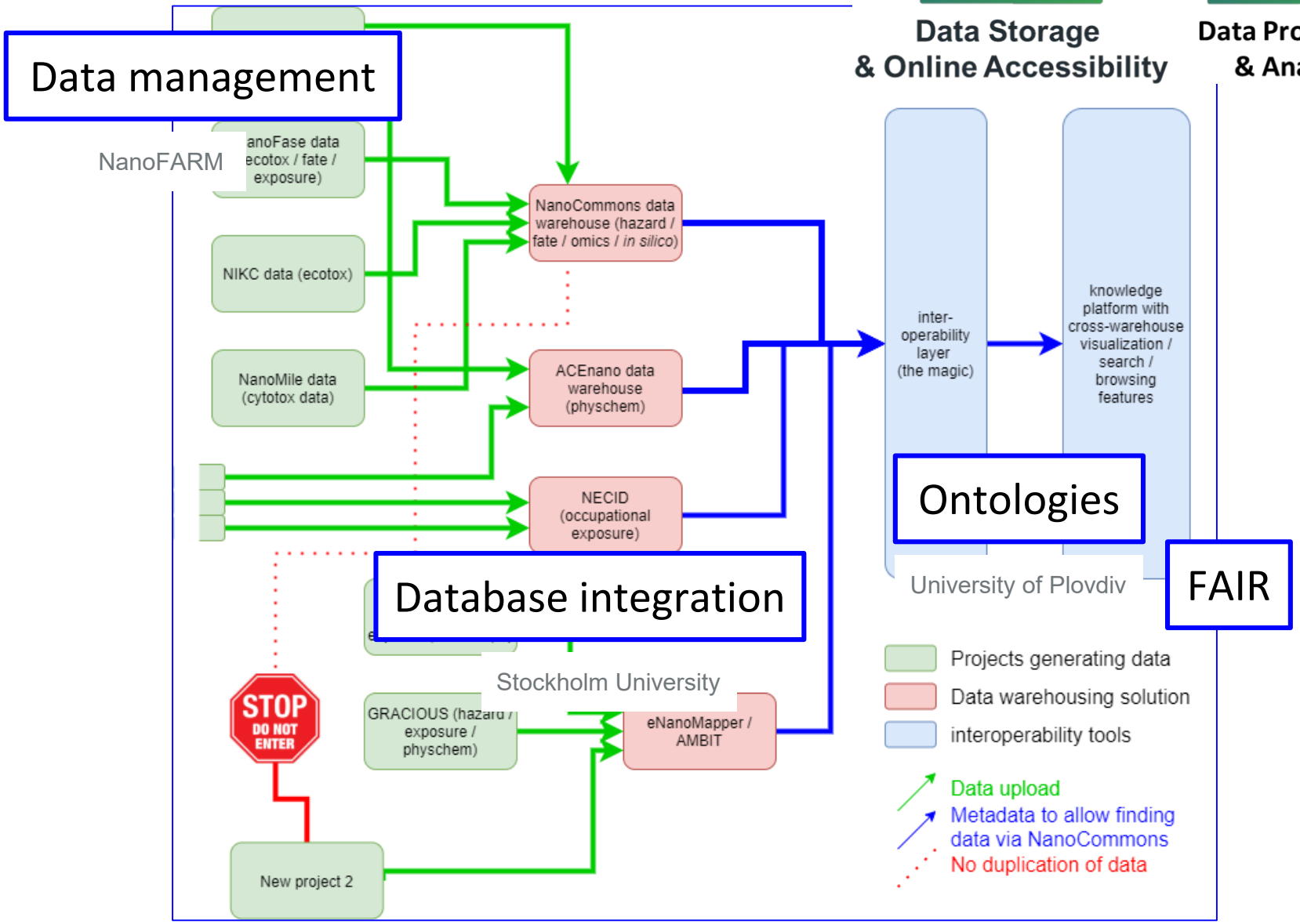
Curation workflows / metadata standards



Electronic lab notebooks



Data sharing



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)

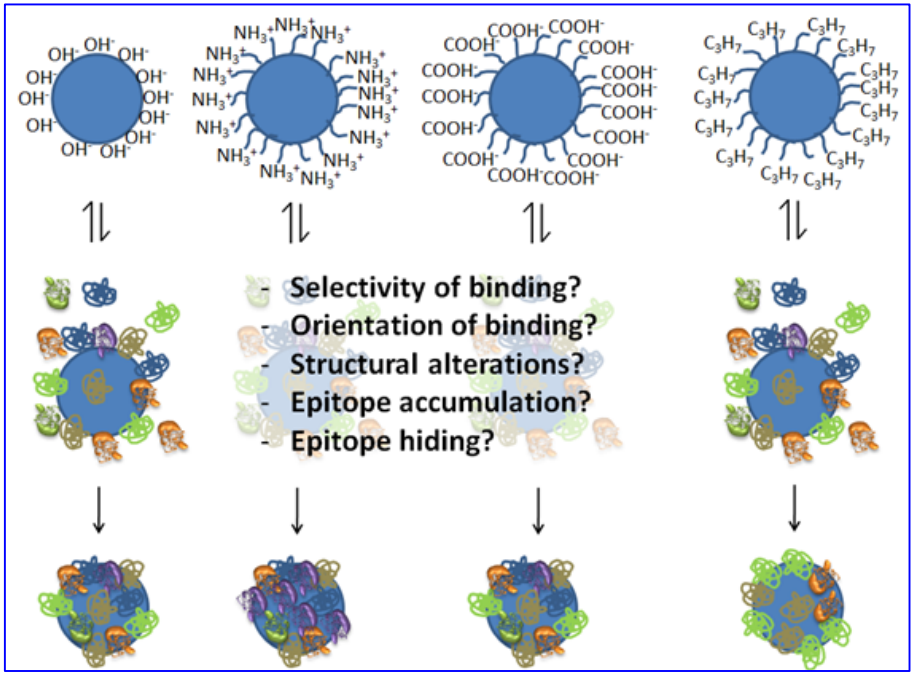
University of Piemonde Orientale (Mesothelioma Expression Profiling)

University of Nevada (PBPK)

Data Processing & Analysis

Data Visualisation & Predictive Toxicity

Data Storage & Online Accessibility



TA: Diamond SARS-CoV-2 Mpro fragment screening program

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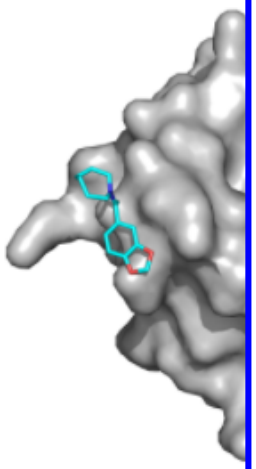
XChem fragment screen

The initial screen encompassed multiple fragment libraries: the DSI-poised library, MiniFrags (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 interes
views here:

- 23 non-covalent hits in the a
- 48 covalent hits in the active
- 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 (t½), 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
t½ (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
t½ <3; >48 h

Good
t½ 8-24 h

t½ 3-8; 24-48 h

For oral dosing (once daily)

Poor If
F <0.4 or t½ <3; >48 h or fdiss <0.7

Good If
F >0.7 and t½ 8-24 h and fdiss >0.85

If
Any other result

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Thank you!

Please remember / post your questions