

The odyssey of data curation

... Or how to make curation fun and
promote data harmonisation

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CENTRE EUROPÉEN
DE RECHERCHE ET D'ENSEIGNEMENT
DES GÉOSCIENCES DE L'ENVIRONNEMENT

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Center for the Environmental
Implications of NanoTechnology

Our Vision

- Implement data management in scientific research
- Data harmonisation through data curation
- Promote data comparability and continuity
- Advance NanoInformatics
- Translational research
- Certification of Curation
- FAIR* access

*FAIR: Findable, Accessible, Interoperable, and Re-usable

Creating Interoperability through Data Curation

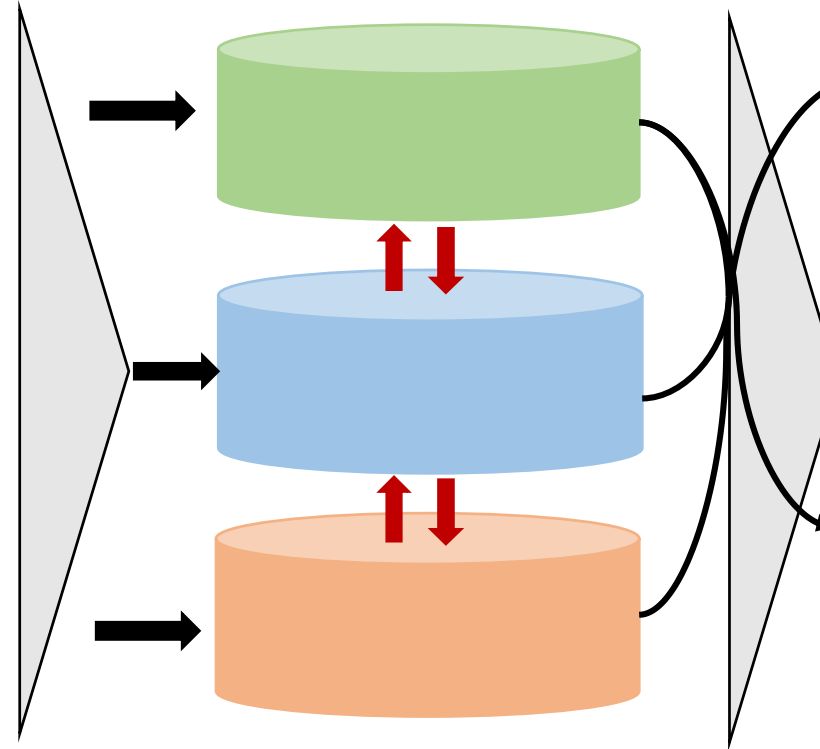
Leverage Diverse Datasets



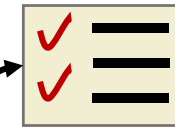
Standard Curation Format



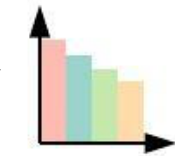
Promote Interoperability



Diverse Data Application



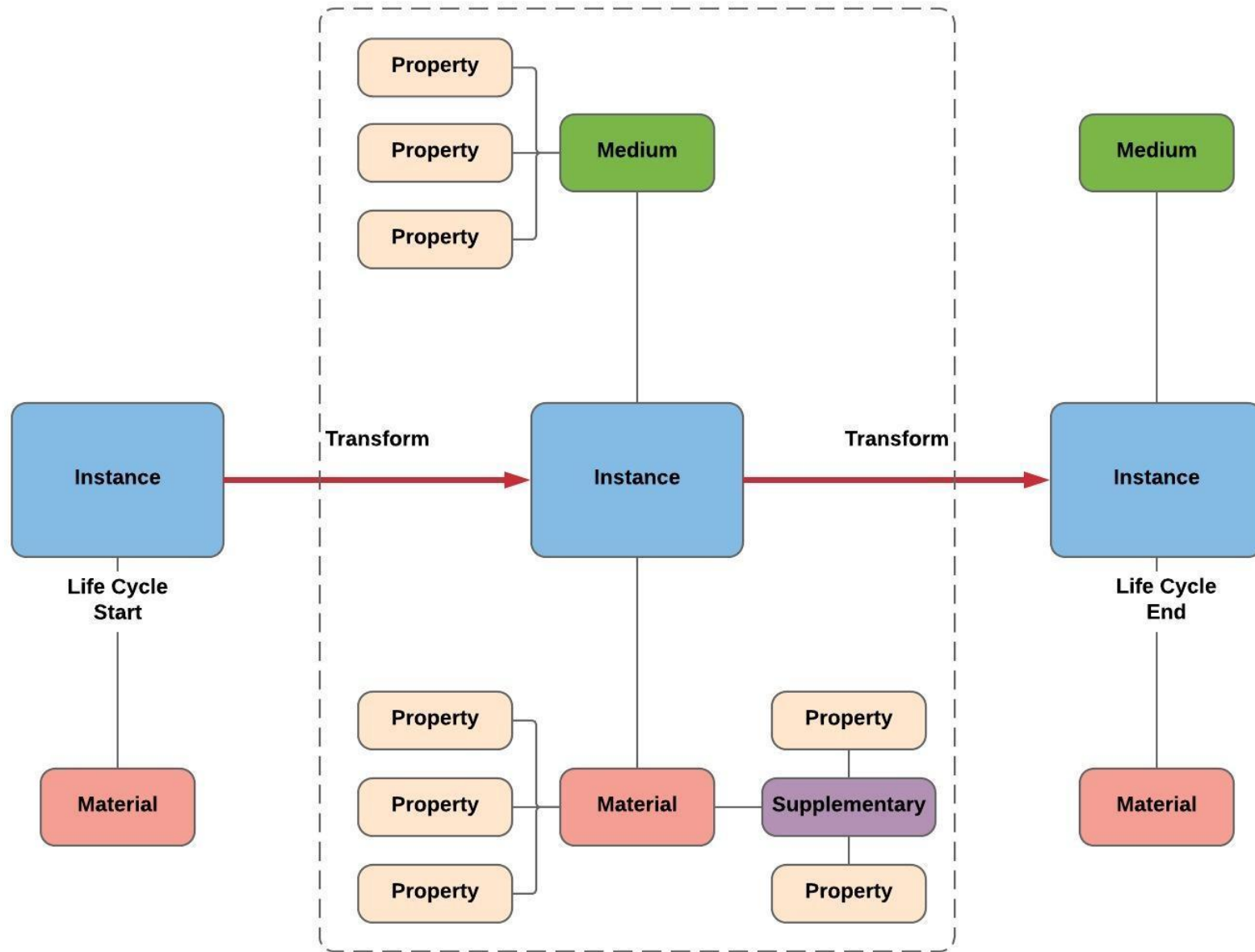
Regulation



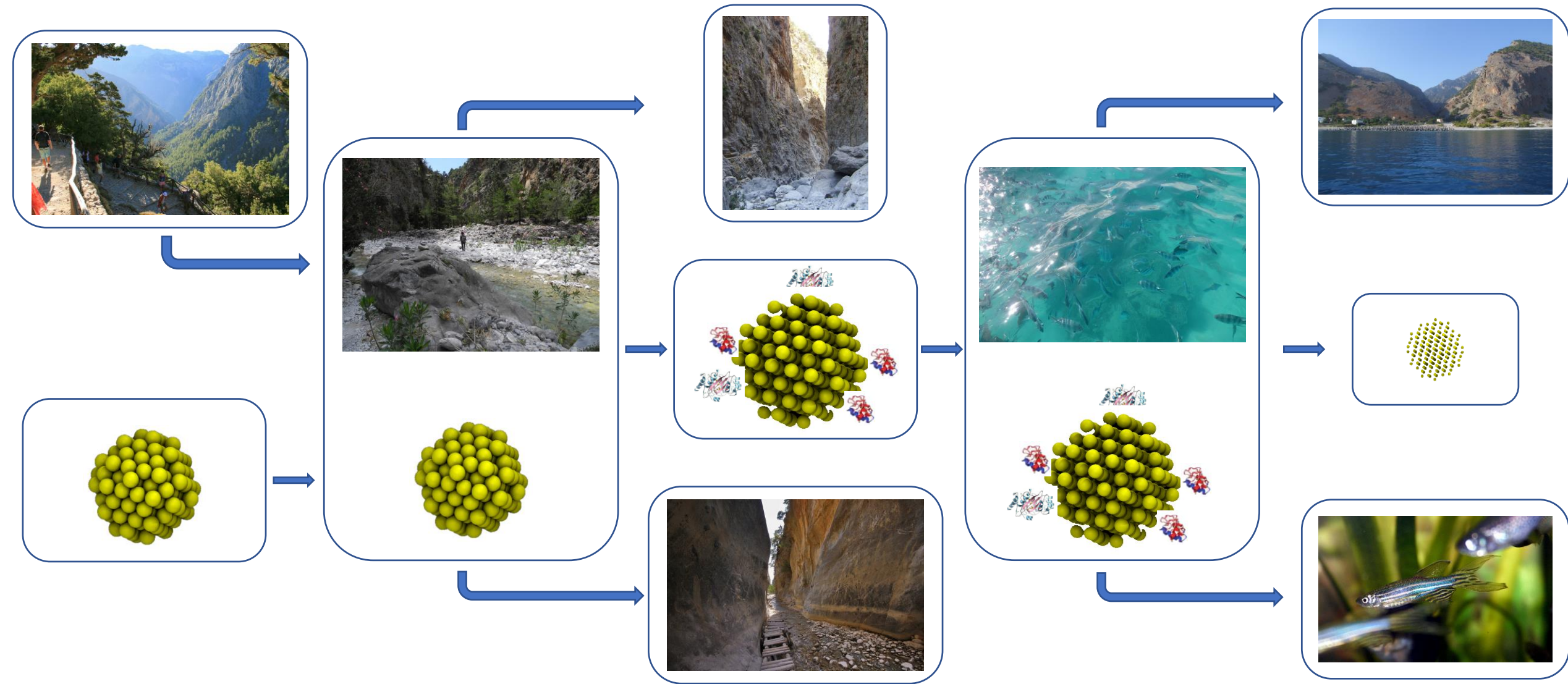
Fate
Exposure
Risk Assessment
Modelling
Data management

- Bridge different fields by promoting data comparability and project continuity
- Shift curation focus from coordinators to data generators

NIKC Instance Organisation Structure

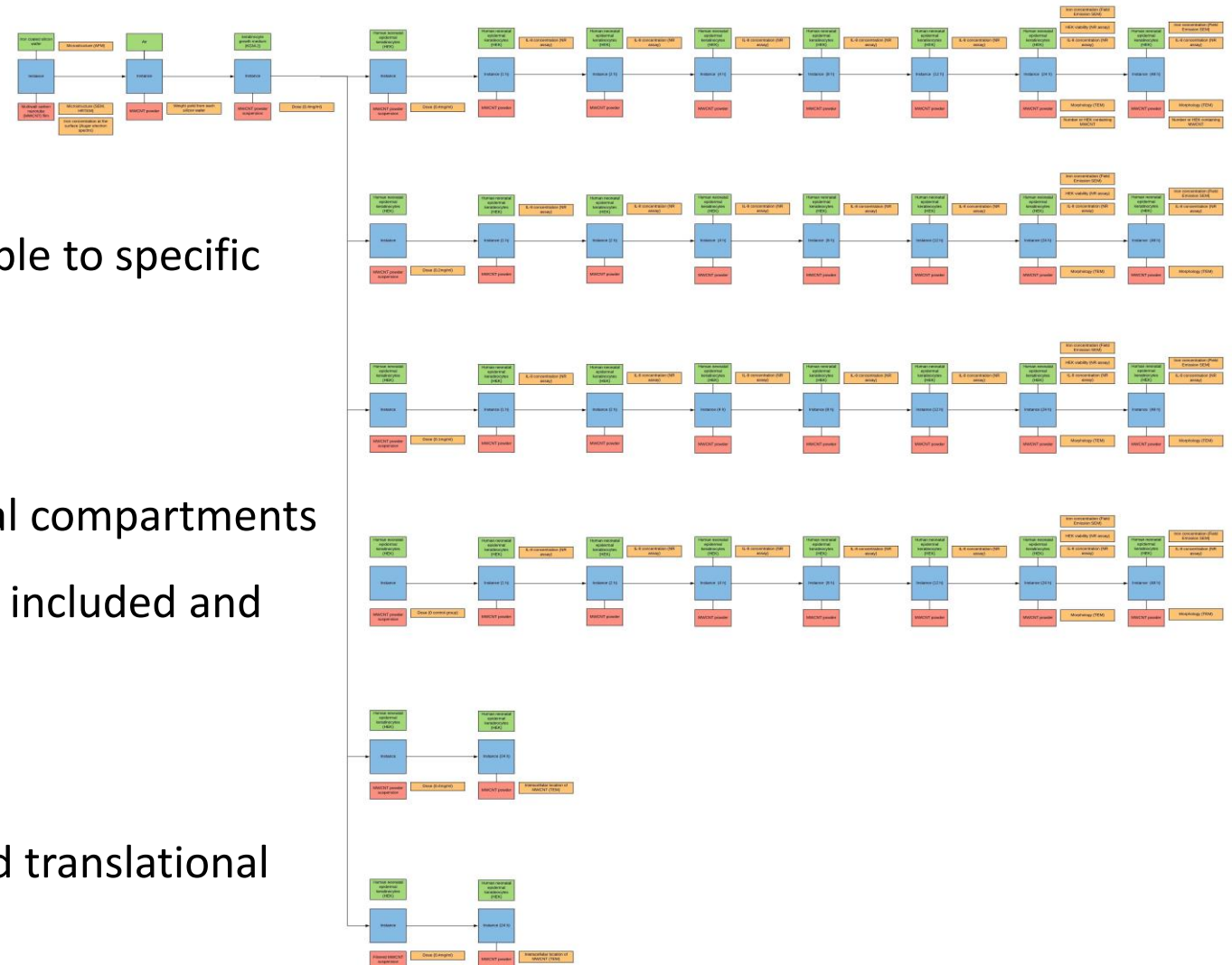


NIKC Instance in Snapshots

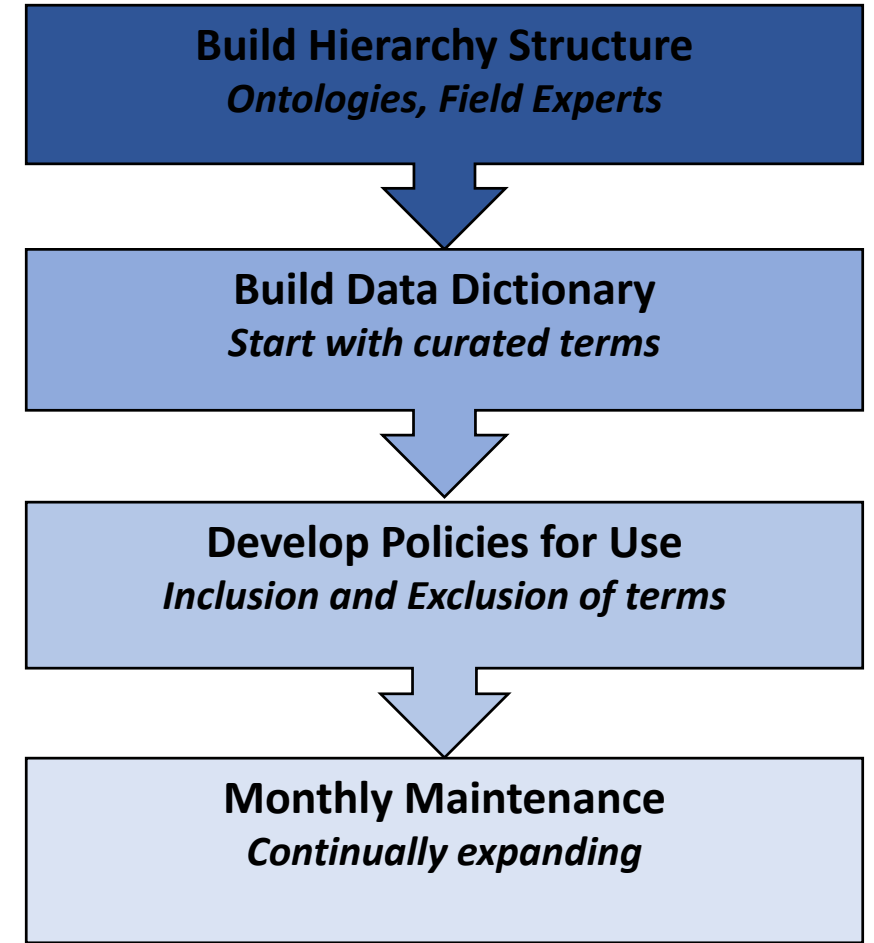
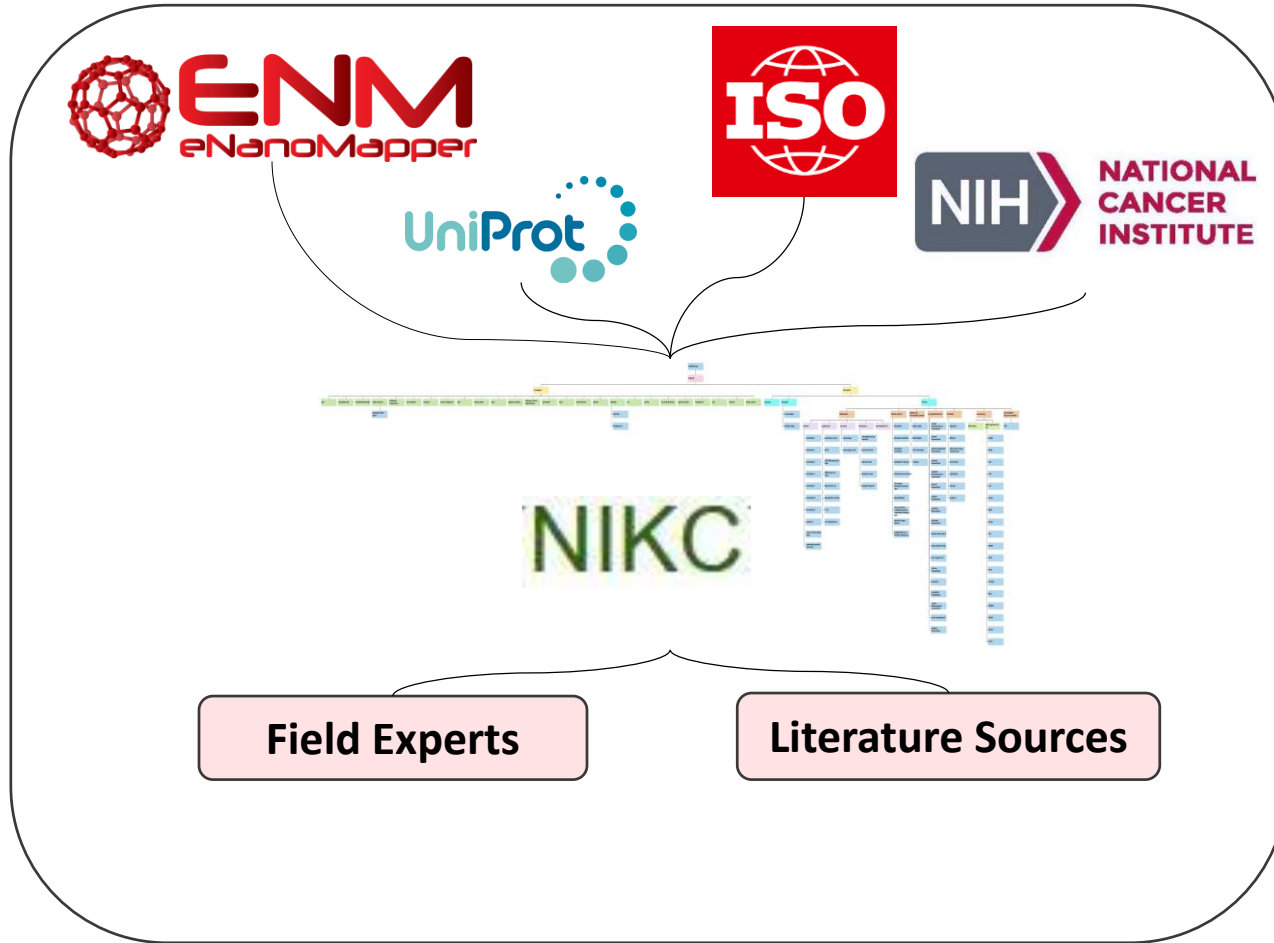


Instance Map: A Transformational Story

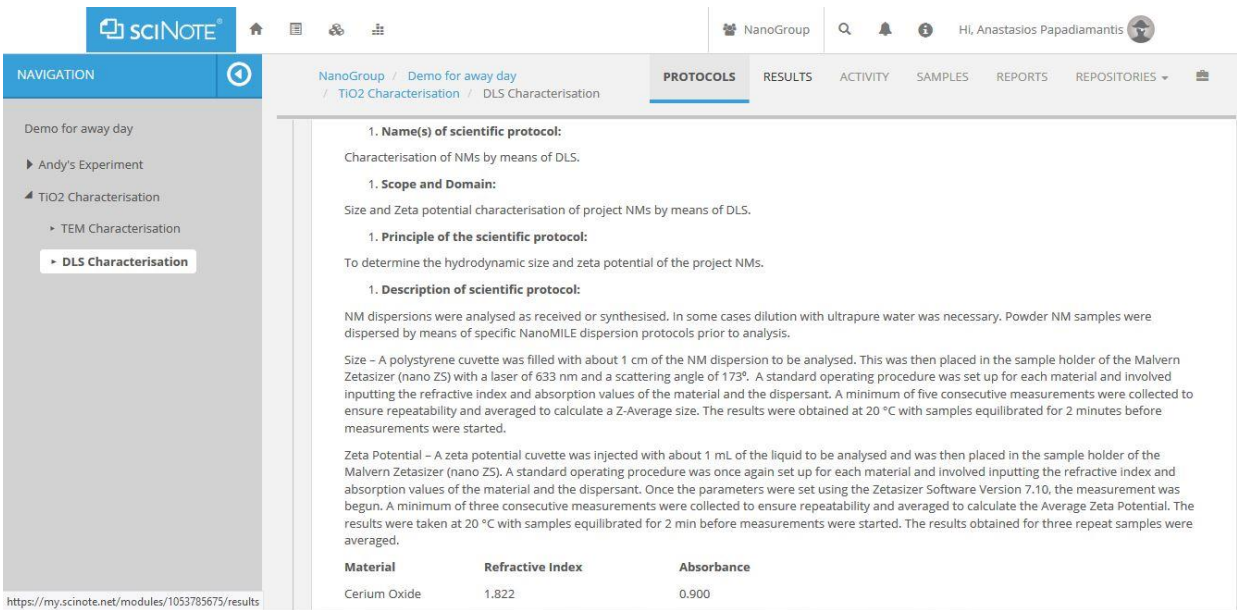
- Dynamic and versatile data templates, adaptable to specific WP requirements
- Common starting point (ENM physicochemical characterisation), connecting all environmental compartments
- Experimental protocols and instruments types included and considered as data points
- Compatible with online lab-books
- Promoting cross-study data harmonisation and translational research



Building a Data Dictionary



Data Management – Online Lab-Books



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NanoGroup / Demo for away day / TIO2 Characterisation / DLS Characterisation

PROTOCOLS RESULTS ACTIVITY SAMPLES REPORTS REPOSITORIES

Demo for away day

► Andy's Experiment

► TIO2 Characterisation

► TEM Characterisation

► **DLS Characterisation**

1. Name(s) of scientific protocol:
Characterisation of NMs by means of DLS.

1. Scope and Domain:
Size and Zeta potential characterisation of project NMs by means of DLS.

1. Principle of the scientific protocol:
To determine the hydrodynamic size and zeta potential of the project NMs.

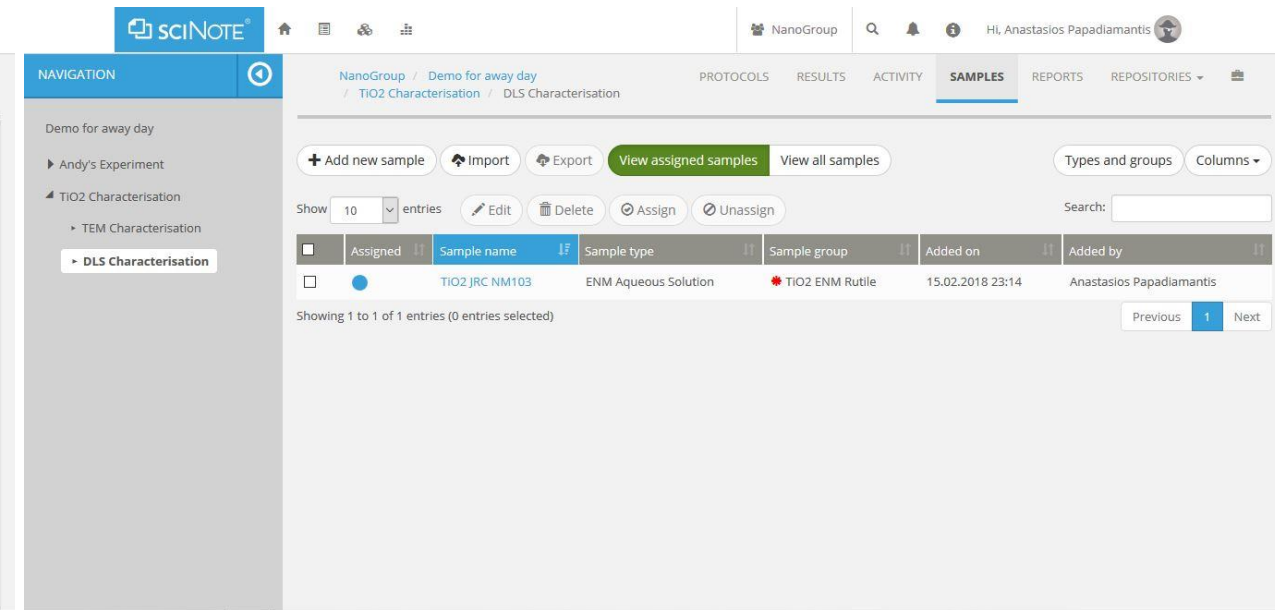
1. Description of scientific protocol:
NM dispersions were analysed as received or synthesised. In some cases dilution with ultrapure water was necessary. Powder NM samples were dispersed by means of specific NanoMILE dispersion protocols prior to analysis.

Size – A polystyrene cuvette was filled with about 1 cm of the NM dispersion to be analysed. This was then placed in the sample holder of the Malvern Zetasizer (nano ZS) with a laser of 633 nm and a scattering angle of 173°. A standard operating procedure was set up for each material and involved inputting the refractive index and absorption values of the material and the dispersant. A minimum of five consecutive measurements were collected to ensure repeatability and averaged to calculate a Z-Average size. The results were obtained at 20 °C with samples equilibrated for 2 minutes before measurements were started.

Zeta Potential – A zeta potential cuvette was injected with about 1 mL of the liquid to be analysed and was then placed in the sample holder of the Malvern Zetasizer (nano ZS). A standard operating procedure was once again set up for each material and involved inputting the refractive index and absorption values of the material and the dispersant. Once the parameters were set using the Zetasizer Software Version 7.10, the measurement was begun. A minimum of three consecutive measurements were collected to ensure repeatability and averaged to calculate the Average Zeta Potential. The results were taken at 20 °C with samples equilibrated for 2 min before measurements were started. The results obtained for three repeat samples were averaged.

Material	Refractive Index	Absorbance
Cerium Oxide	1.822	0.900

<https://my.scinote.net/modules/1053785675/results>



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SAMPLES PROTOCOLS RESULTS ACTIVITY REPORTS REPOSITORIES

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+ Add new sample Import Export View assigned samples View all samples

Show 10 entries Edit Delete Assign Unassign

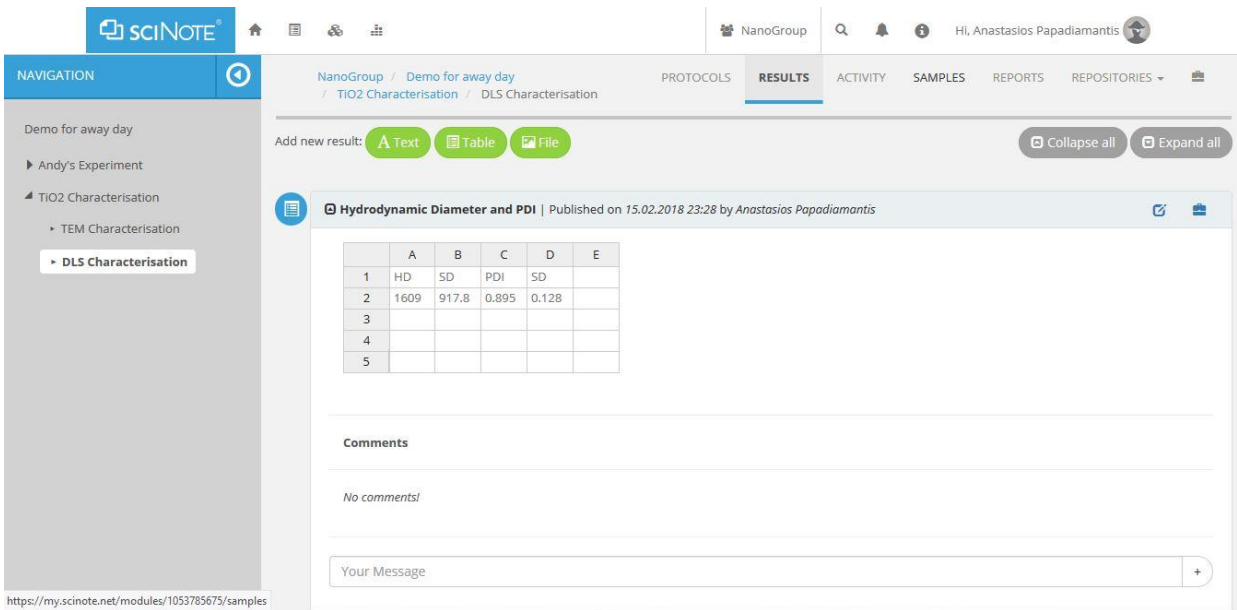
Types and groups Columns

Search:

Assigned	Sample name	Sample type	Sample group	Added on	Added by
<input type="checkbox"/>	TIO2 JRC NM103	ENM Aqueous Solution	TIO2 ENM Rutile	15.02.2018 23:14	Anastasios Papadimitris

Showing 1 to 1 of 1 entries (0 entries selected)

Previous 1 Next



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Add new result: Text Table File Collapse all Expand all

Hydrodynamic Diameter and PDI | Published on 15.02.2018 23:28 by Anastasios Papadimitris

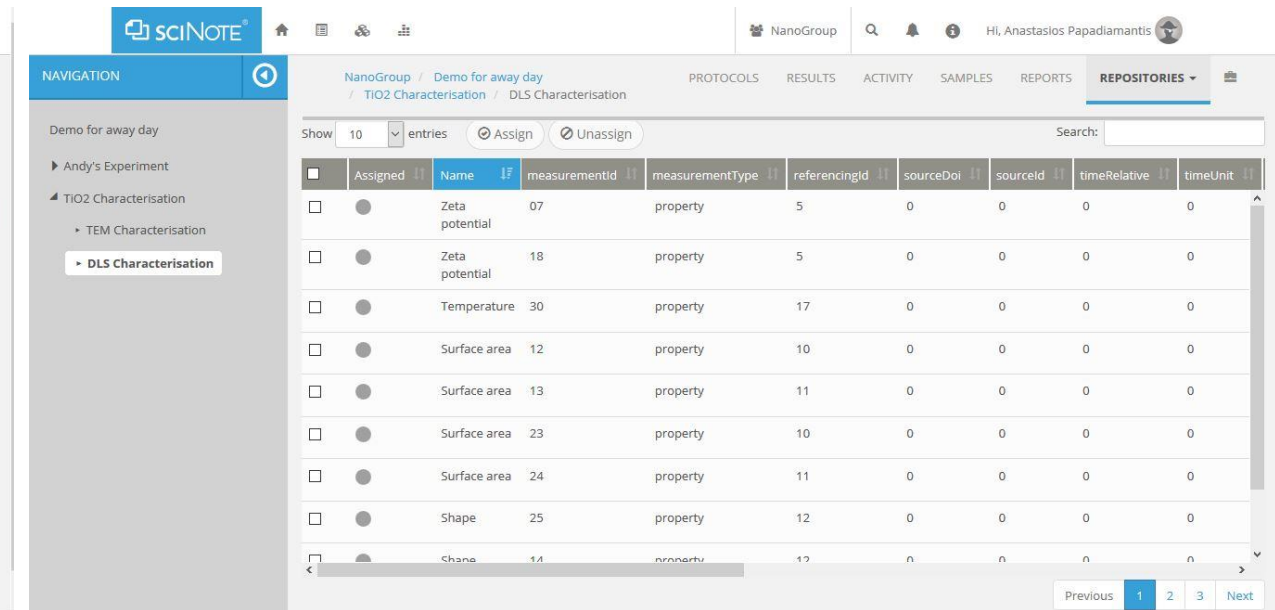
	A	B	C	D	E
1	HD	SD	PDI	SD	
2	1609	917.8	0.895	0.128	
3					
4					
5					

Comments

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Show 10 entries Assign Unassign

Search:

Assigned	Name	measurementId	measurementType	referencingId	sourceDoi	sourceId	timeRelative	timeUnit
<input type="checkbox"/>	Zeta potential	07	property	5	0	0	0	0
<input type="checkbox"/>	Zeta potential	18	property	5	0	0	0	0
<input type="checkbox"/>	Temperature	30	property	17	0	0	0	0
<input type="checkbox"/>	Surface area	12	property	10	0	0	0	0
<input type="checkbox"/>	Surface area	13	property	11	0	0	0	0
<input type="checkbox"/>	Surface area	23	property	10	0	0	0	0
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<input type="checkbox"/>	Shape	25	property	12	0	0	0	0
<input type="checkbox"/>	Shape	14	property	12	0	0	0	0

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Steps to fulfill our vision

- Shift curation onto data generators
- Electronic laboratory notebooks with implemented NIKC compatible curation templates
- Automated dataset extraction and uploading
- Create an open and dynamic data repository, implement visualisation and analysis tools
- Use the curated data to address all topics of nanosafety research (risk assessment, exposure, fate, safer-by-design, regulatory)
- FAIR access

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Marianne Matzke





Thank you for your attention