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

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Nano-Knowledge Community

Data management in nanosafety research: From bench to database thus streamlining analysis and publication

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Overview

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1. **Data Management and Data Lifecycle**
2. Data Curation
3. Online Lab-Books
4. Case Studies
5. Conclusions

What is Data Management

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Definition

Data Management is the implementation and application of processes, which allow the acquisition, storage, manipulation and analysis of data during its lifecycle.

Scope

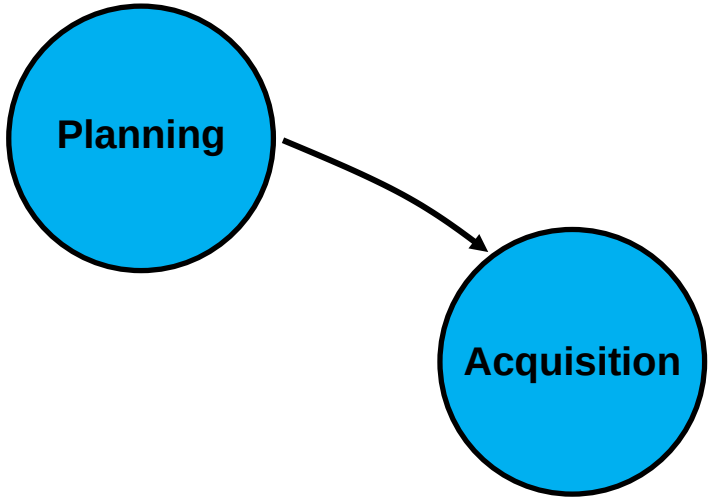
- Implement data management in scientific research
- Promote data harmonisation through data curation
- Promote data comparability and continuity
- Advance NanoInformatics
- Translational research
- FAIR* access

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

Data Lifecycle

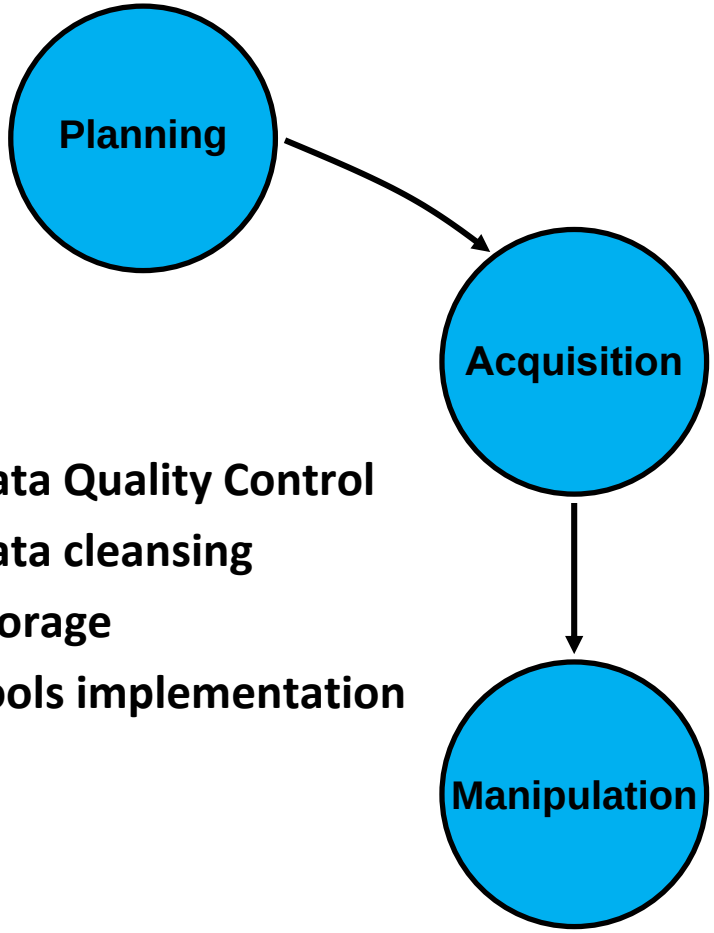
1. Endpoint identification
2. Experimental design
3. Data management plan
4. Data templates creation

Data Lifecycle



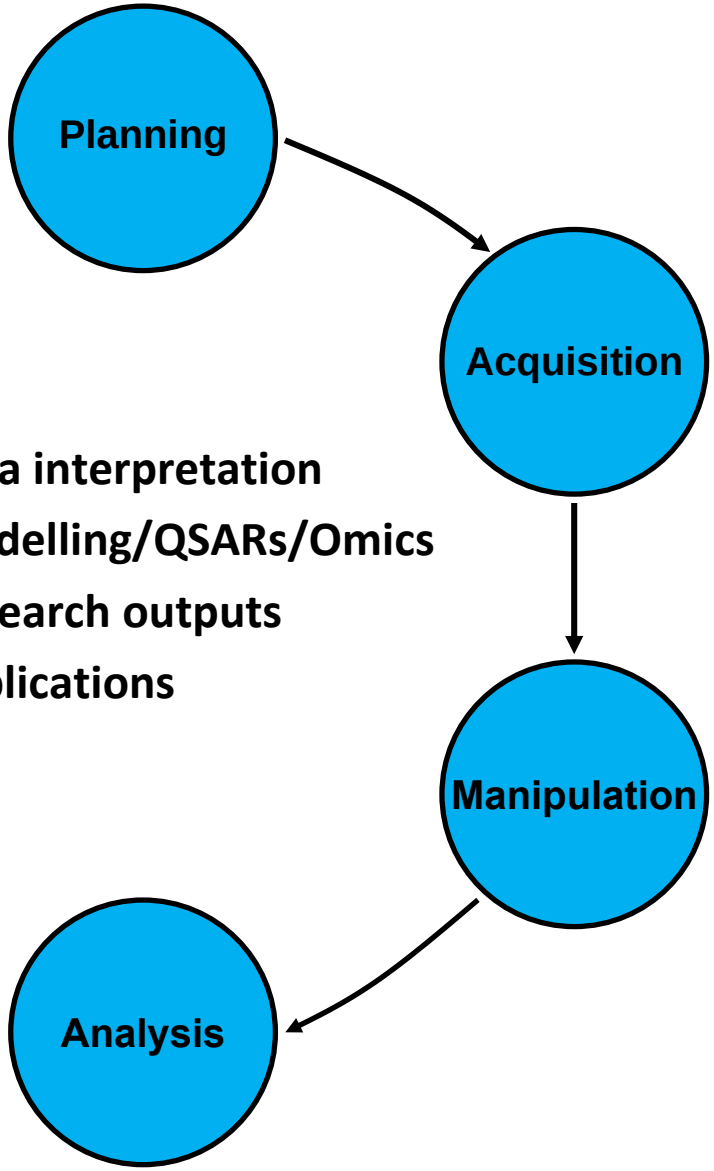
1. Data acquisition
2. Data curation
3. Data digitisation

Data Lifecycle



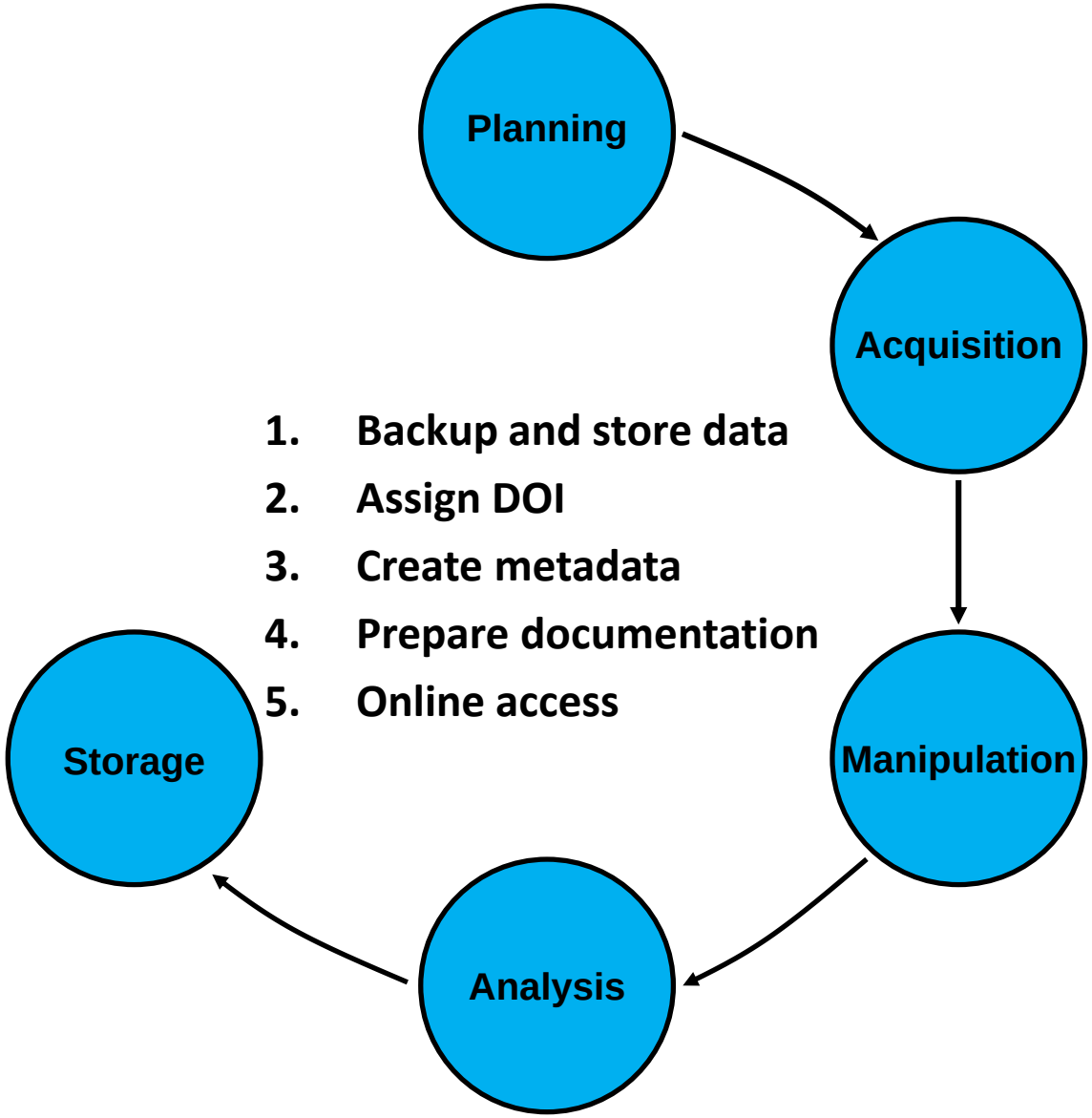
1. Data Quality Control
2. Data cleansing
3. Storage
4. Tools implementation

Data Lifecycle



1. Data interpretation
2. Modelling/QSARs/Omics
3. Research outputs
4. Publications

Data Lifecycle



Data Lifecycle

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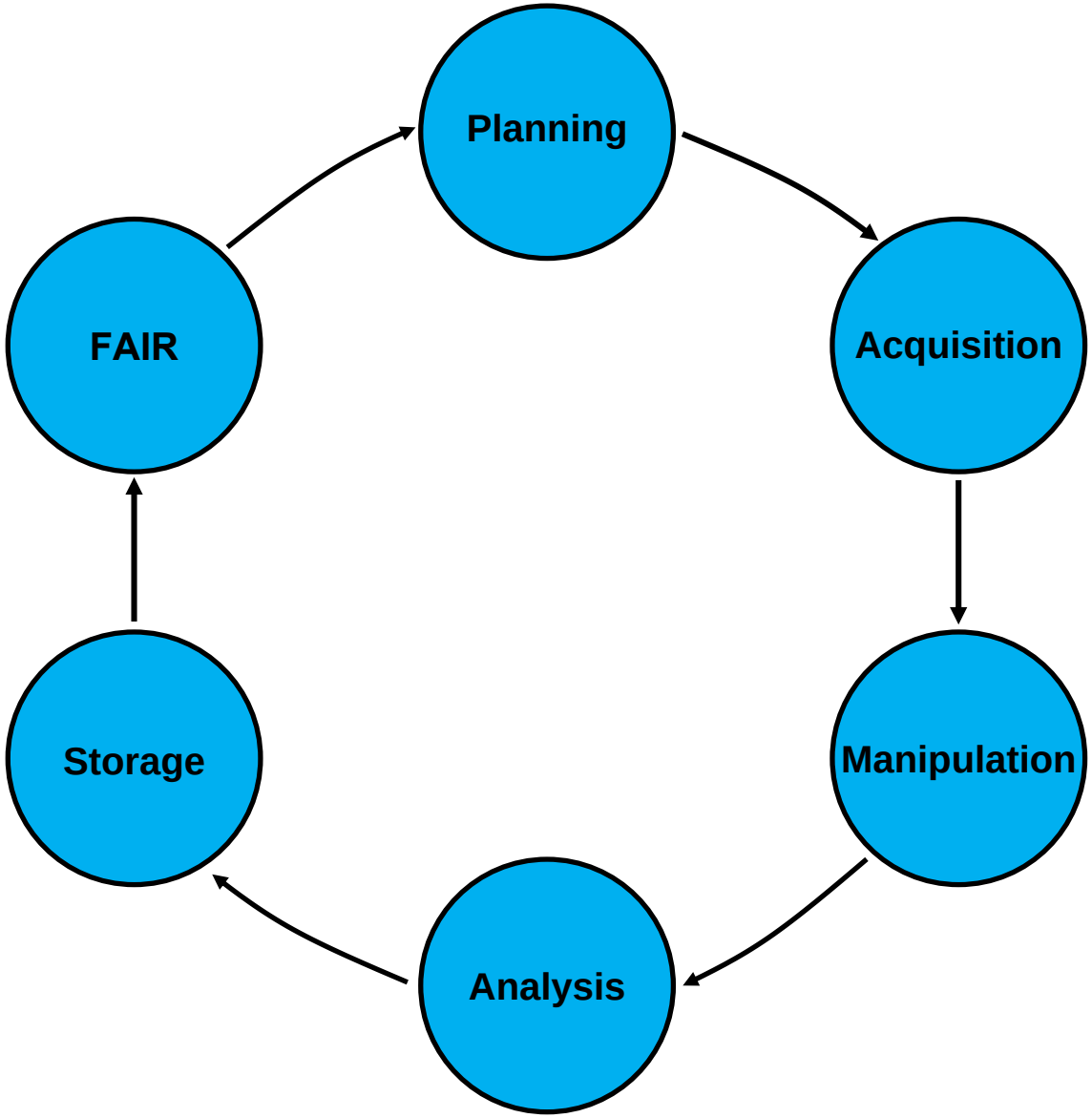

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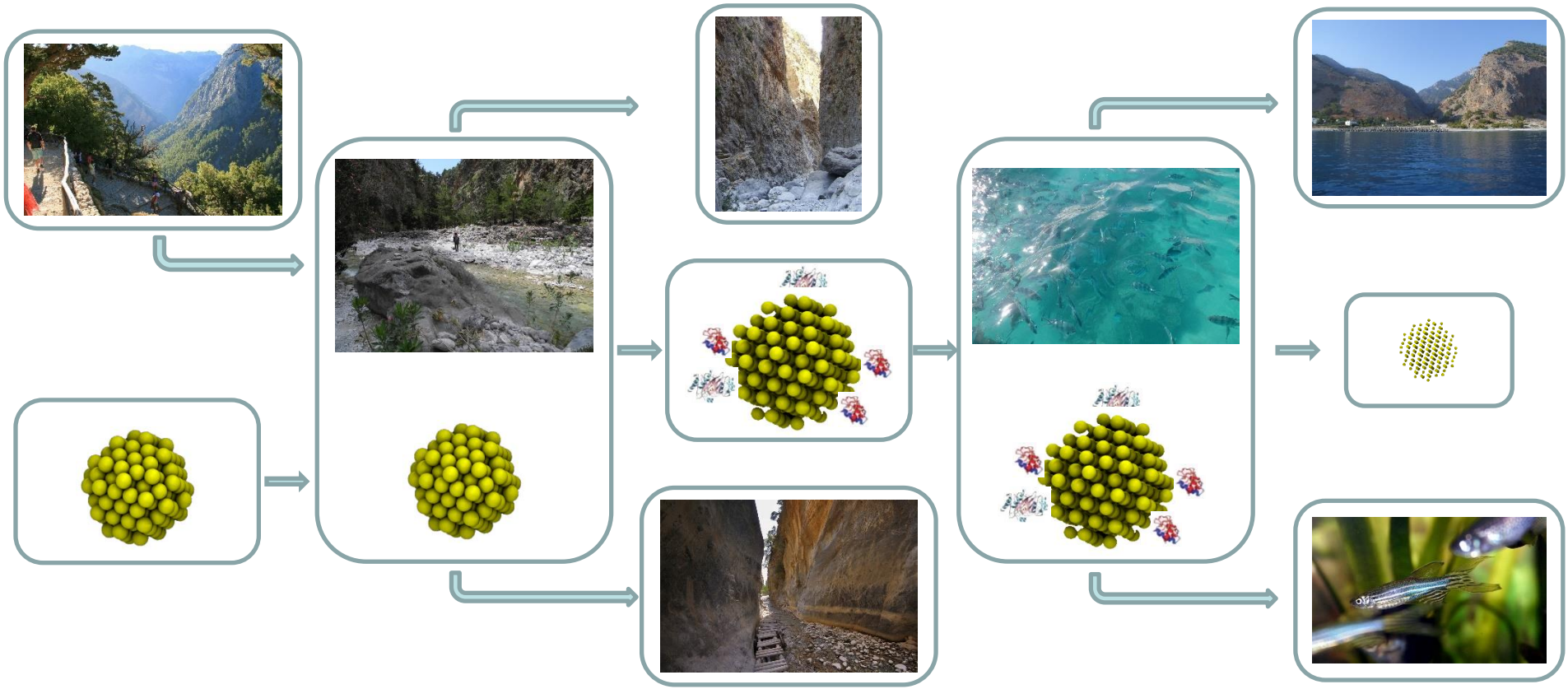
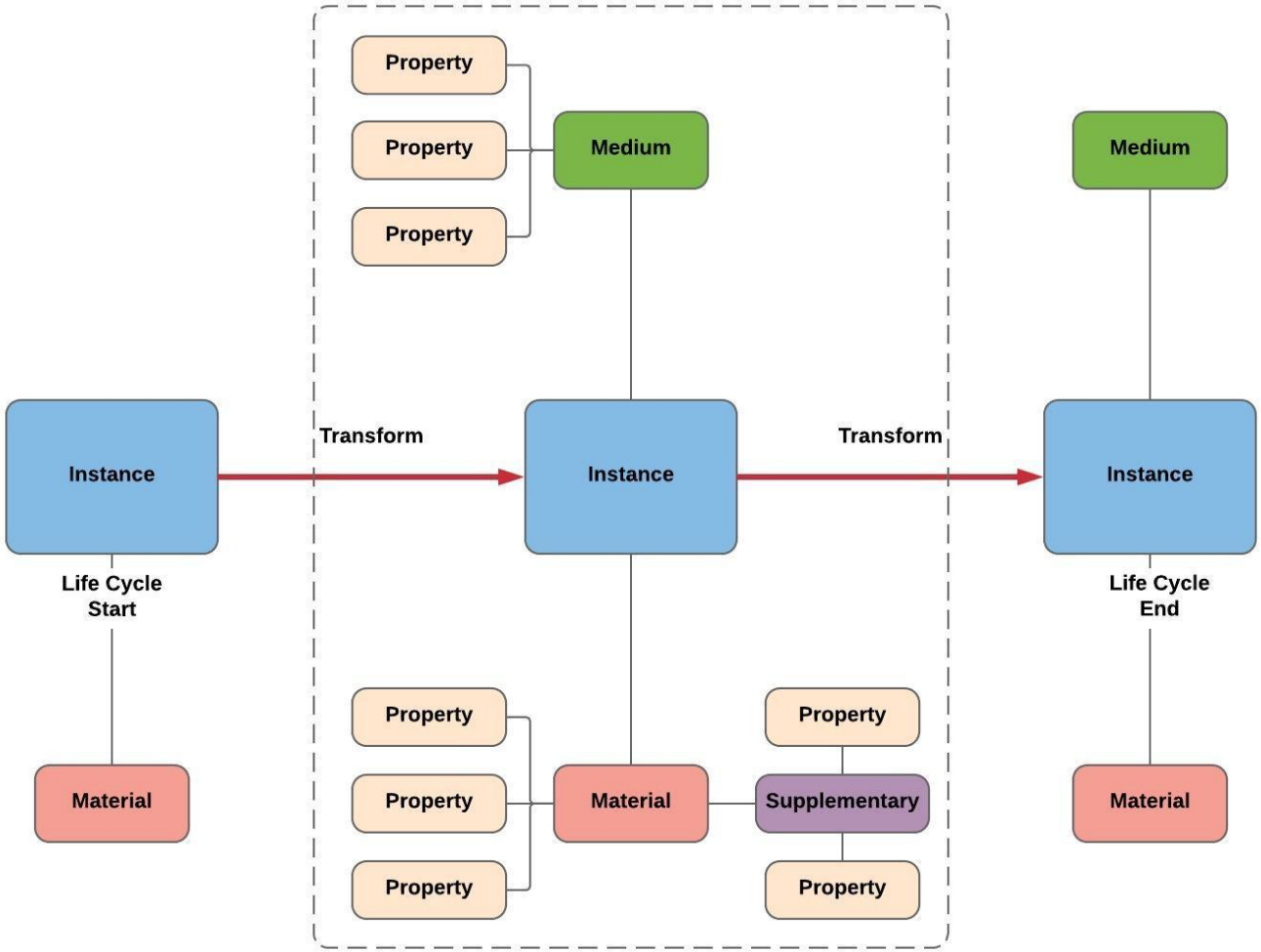
Exposure Case Study



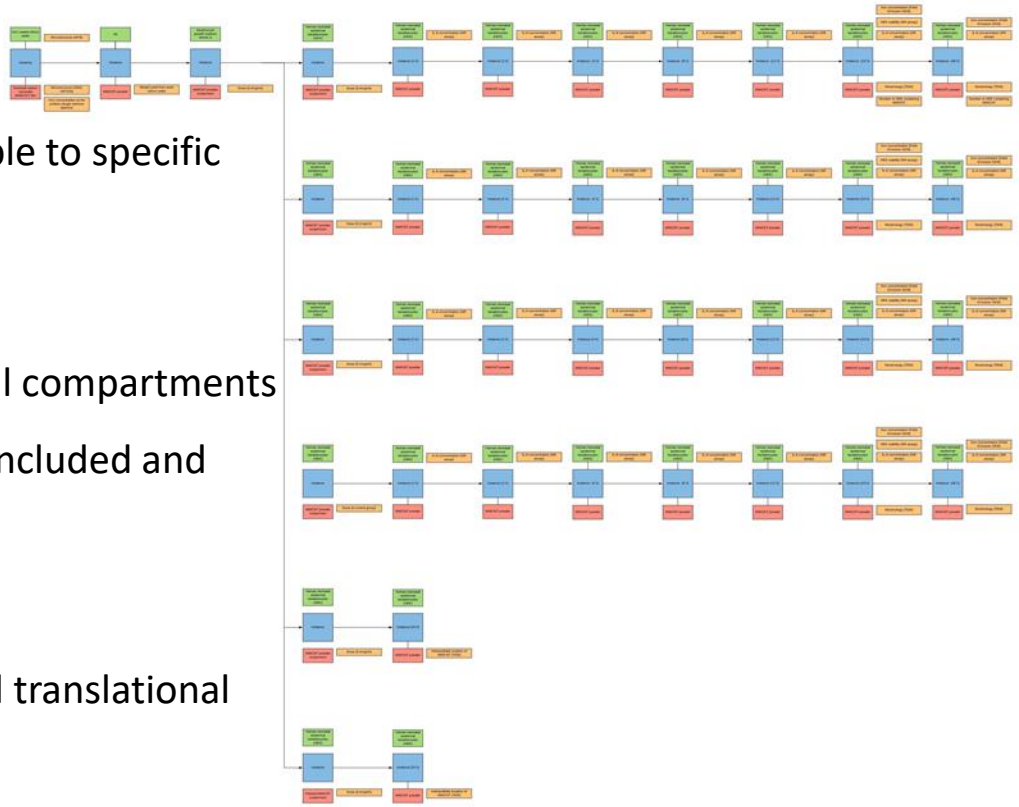
- **A released nanomaterial will change itself and affect its surrounding environment**

Data Curation & NIKC Instance



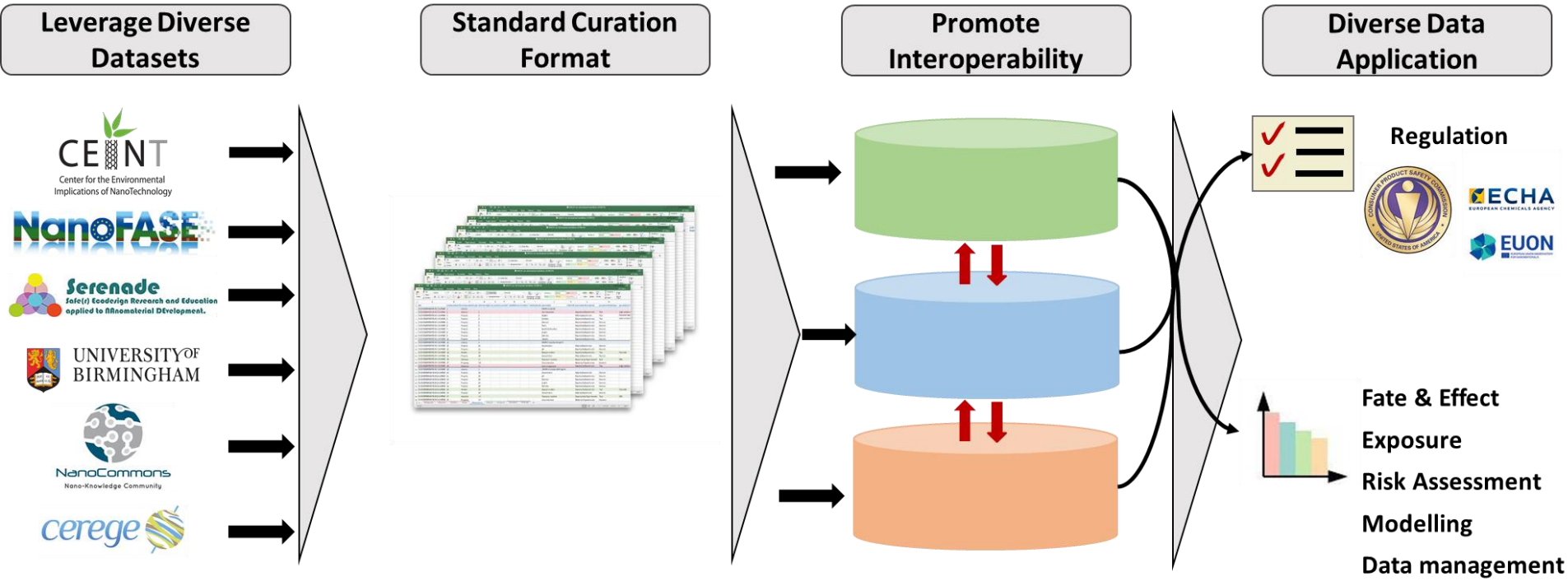
Data Curation: The process of data collection and organisation

Instance Map: Adaptability



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

Data Curation & Interoperability



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

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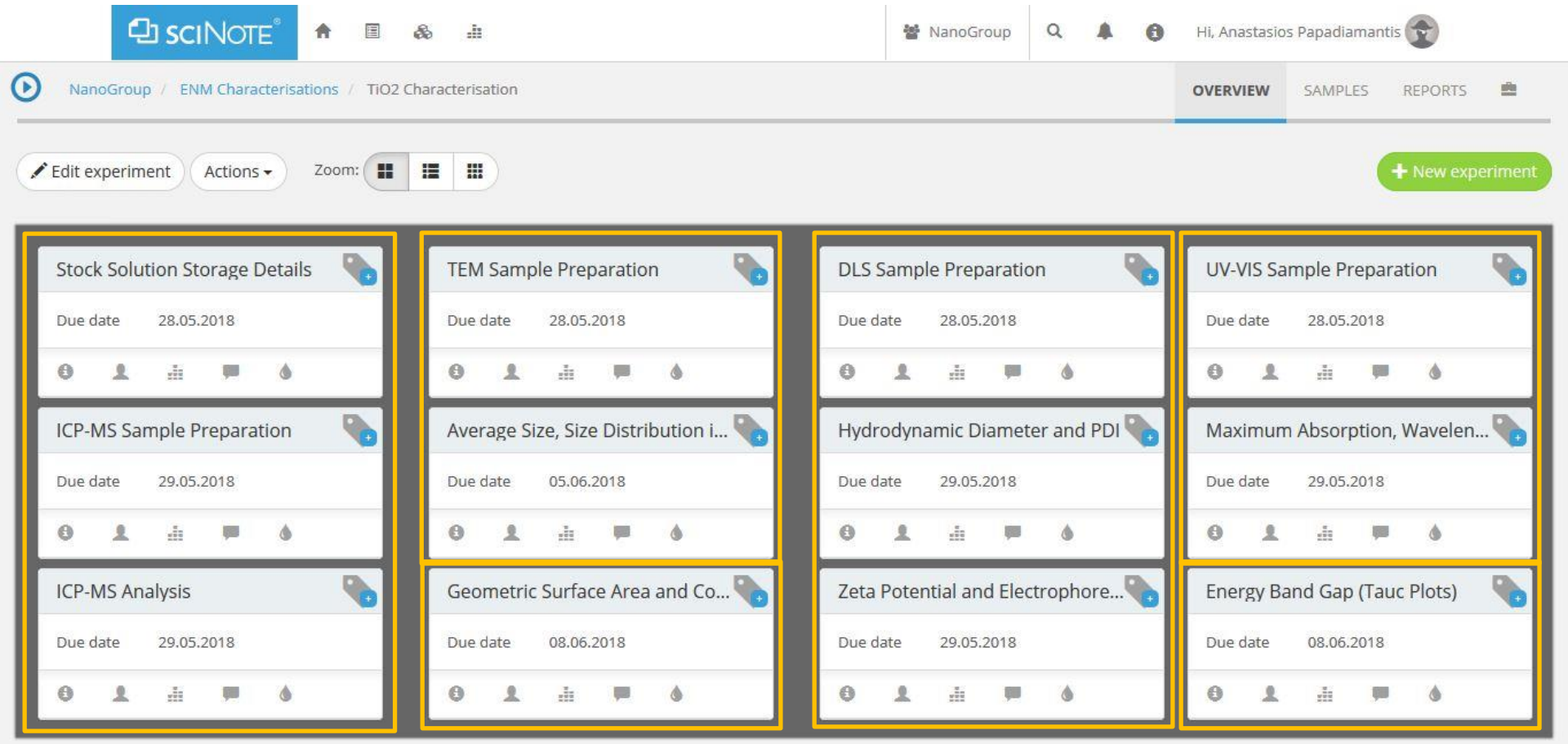
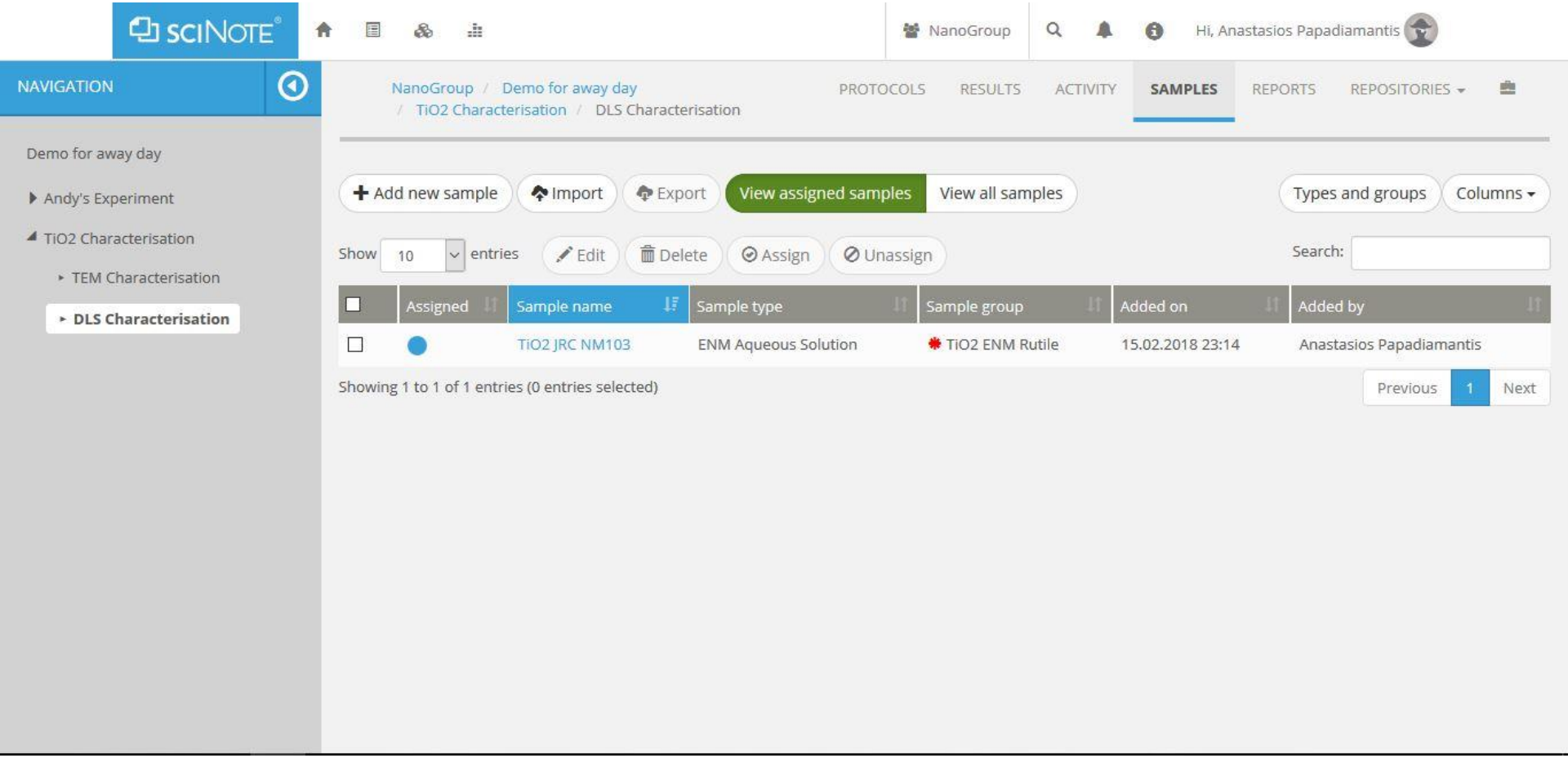
Experimental Workflow



- **Multiple-branch experimental workflows**

Data Acquisition & Management



- **Sample insertion and assignment**

Data Acquisition & Management

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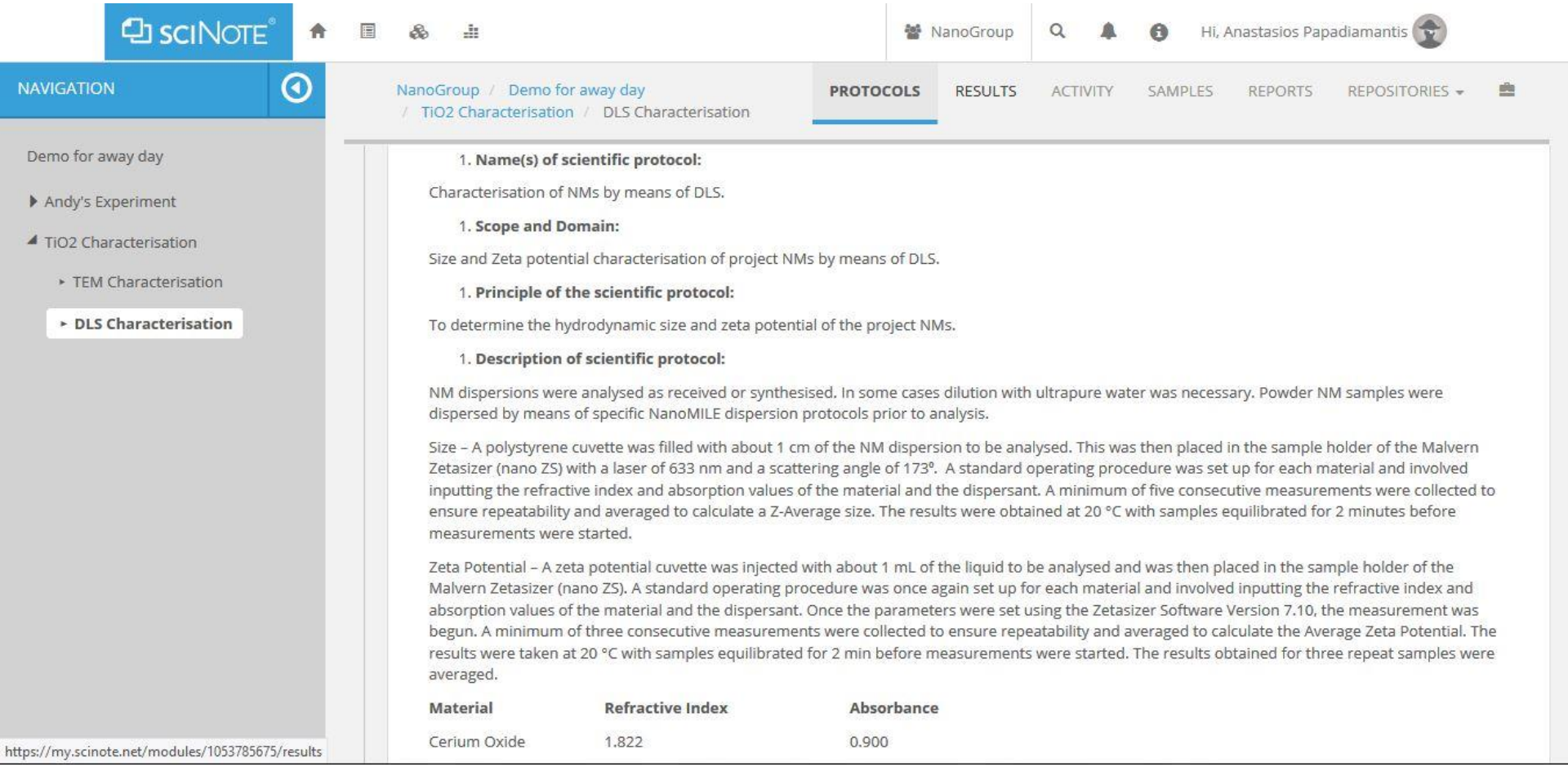
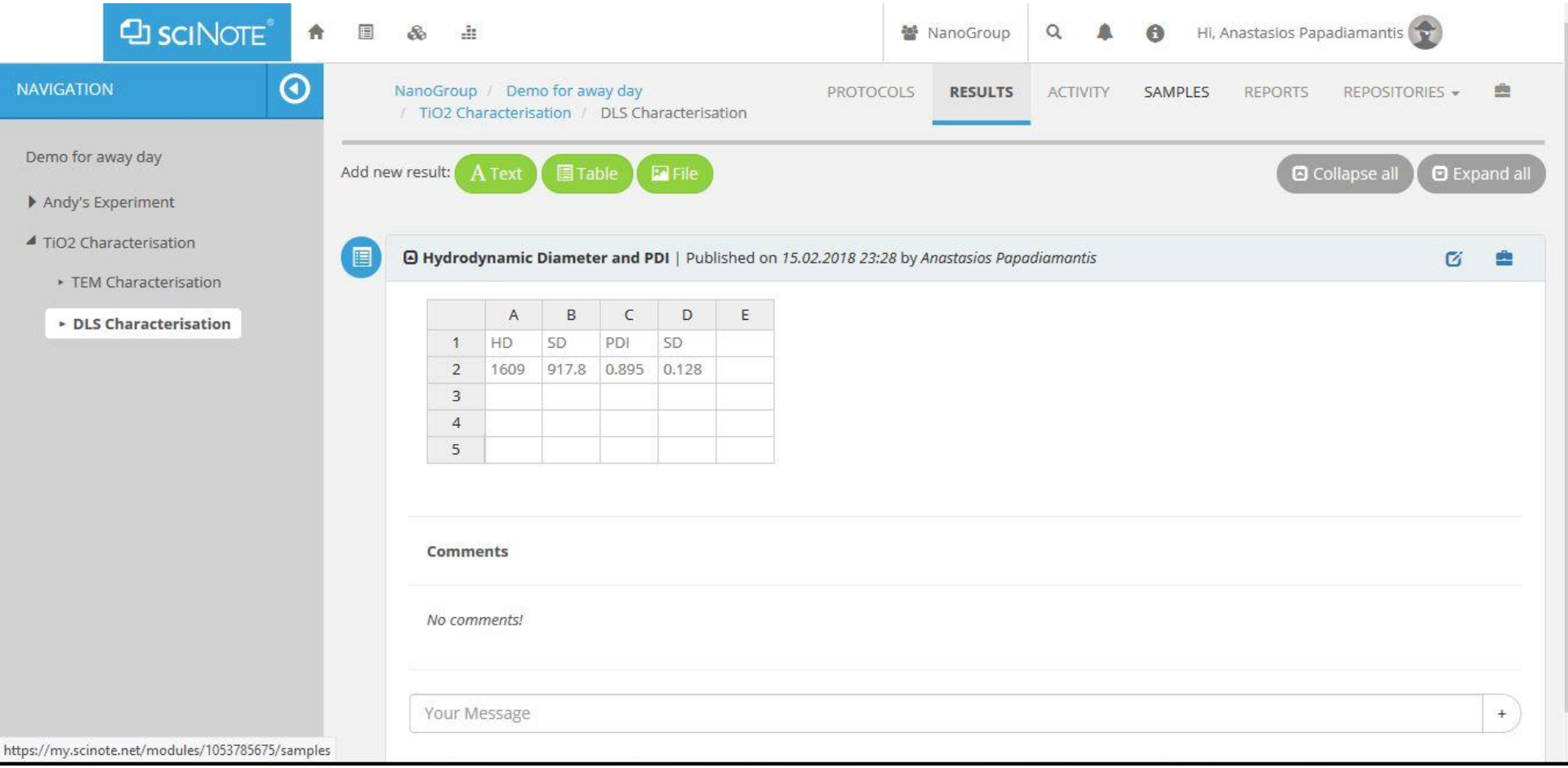


- **Fully linked analytical protocols**

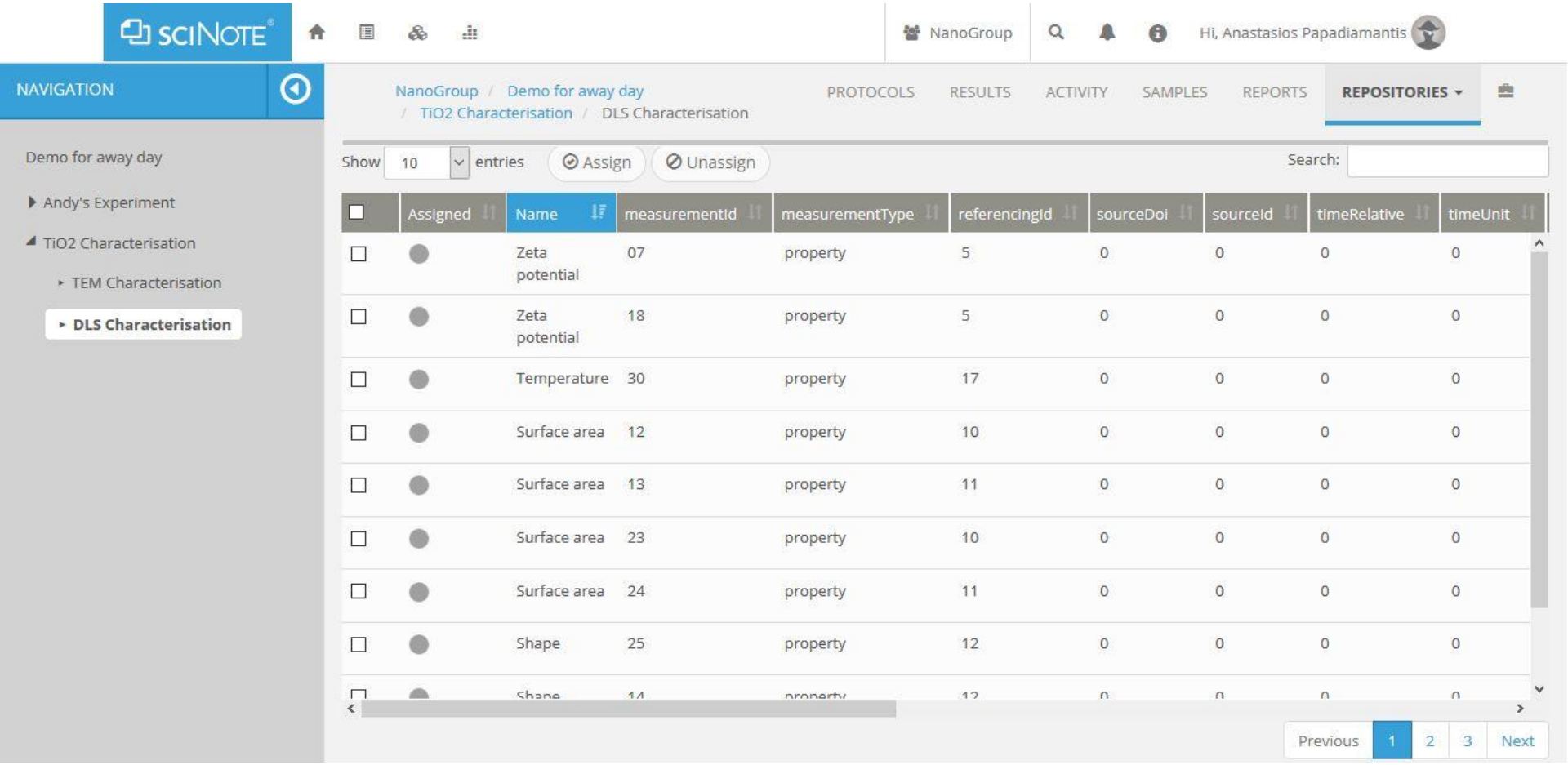
Data Acquisition & Management



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

- **Specific experimental results**

Data Acquisition & Management



- **Direct link to data curation template**
- **Automatic extraction and shipment to data repository via email**

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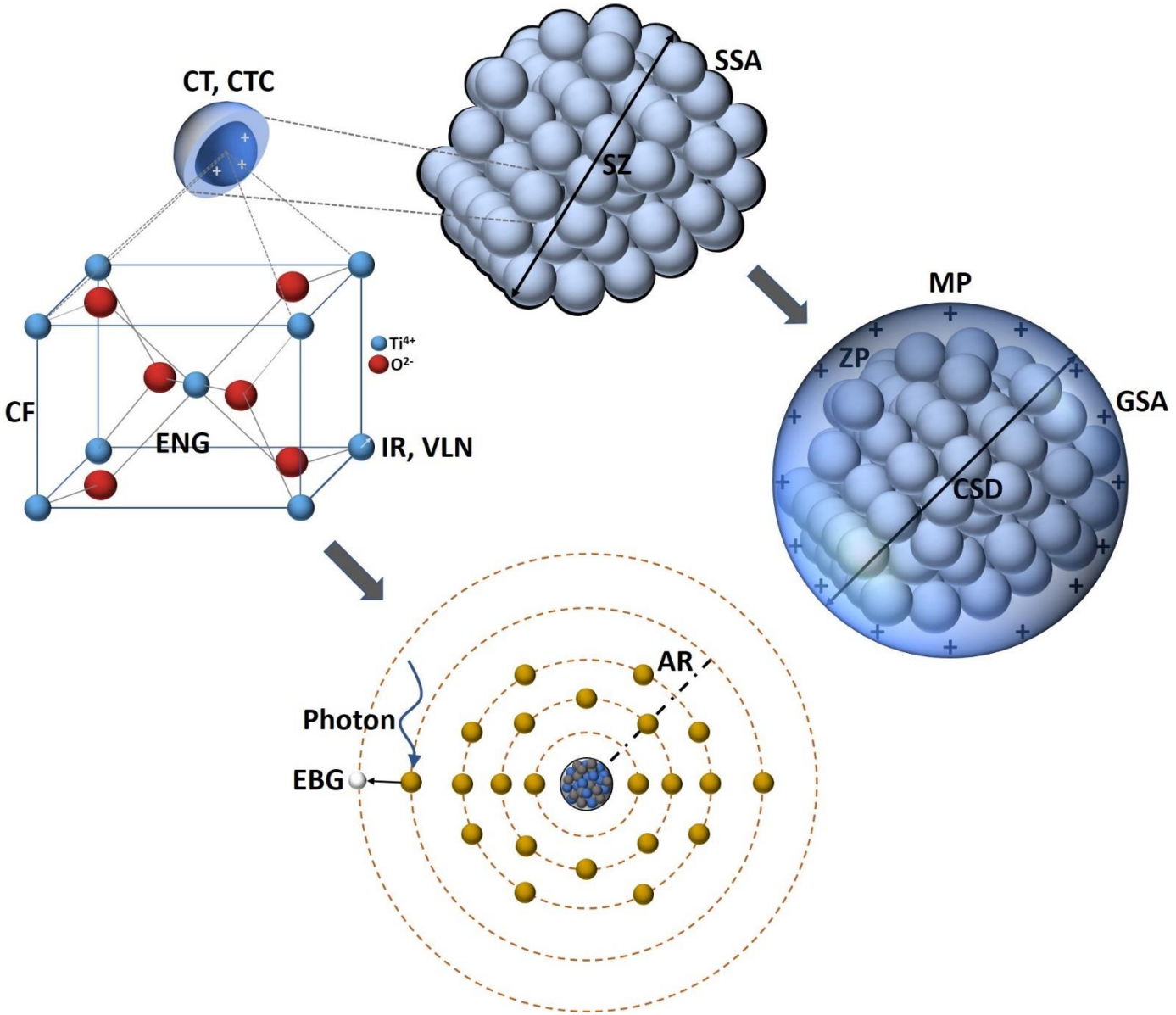
Nanomaterials Characterisation



From a Local Network…

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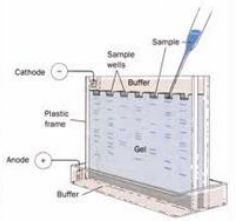
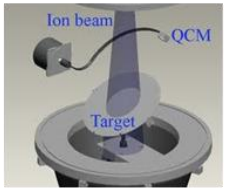
DCS



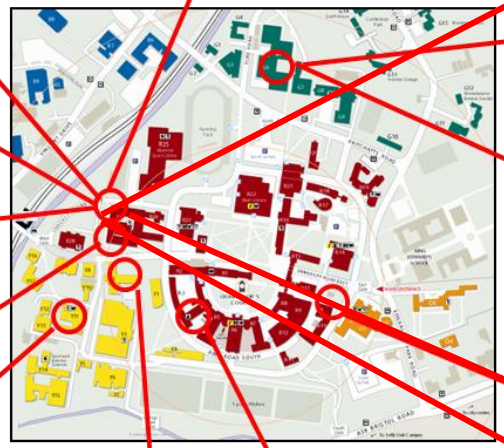


QCM


BET

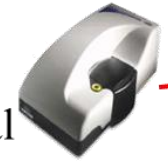
Eco-interactions
(Electrophoresis, gel imaging etc.)

FFF

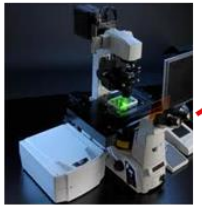



TEM
(+ EDS, EELS)

DLS
Zeta potential

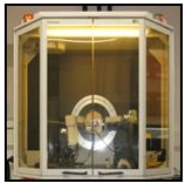



SEM,
ESEM


Confocal


AFM


NTA


XRD


ICP-MS
Sp-ICP-MS
ICP-AES
Sc-ICP-MS


UV-VIS

From a Local Network…

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measurementId	measurementType	referencingId	timeRelative	timeUnit	timeAbsolute	parameter	inheritId	parameterDescription	parameterDataType	parameterText
1	instance				2018-04-23 09:00:00					
2	material	1				core composition			text	ag2s suspension
3	property	2				coating			text	uncoated
4	property	2				nominal diameter			numeric	
5	property	2				morphology			text	
6	property	2				concentration			numeric	
7	property	2				diameter			numeric	
8	property	2				hydrodynamic diameter			numeric	
9	property	2				zeta potential			numeric	
10	property	2				Surface area			numeric	
11	property	2				Corresponding sphere diameter			numeric	
12	property	2				maximum absorption intensity			numeric	
13	property	2				wavelength at maximum absorption			numeric	
14	property	2				energy band gap			numeric	
15	system	1				name			text	Water
16	property	15				temperature		storage temperature	numeric	
17	property	15				pH		storage pH	numeric	

- **As produced data capturing of nanomaterials physicochemical, structural and computational characterisation**

To a Wide Network…

- **Aquatic and terrestrial mesocosm experiment, 7 EU countries and 10 Institutions**

To a Wide Network…

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ID	measurementId	measurementType	referencingId	timeRelative	timeUnit	timeAbsolute	parameter	inheritId	parameterDescription	parameterDataType	parameterText	parameter
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	326	property	25	7	day		Kda Ag		Kda Ag 54	numeric		
	327	property	25	7	day		Kda Ag		Kda Ag 55	numeric		
	328	property	25	7	day		Kda Ag		Kda Ag 56	numeric		
	329	property	25	7	day		Kda Ag		Kda Ag 57	numeric		
	330	property	25	7	day		Kda Ag		Kda Ag 58	numeric		
	331	property	25	7	day		Kda Ag		Kda Ag 59	numeric		
	332	property	25	7	day		Kda Ag		Kda Ag 60	numeric		
	333	property	25	7	day		Kda Ag		average Kda Ag	numeric		
	334	system	21				name			text	soil	
	335	property	334	7	day		diameter		diameter	numeric		
	336	property	334	7	day		diameter		diameter	numeric		
	337	property	334	7	day		diameter		average diameter	numeric		
	338	property	334	7	day		microbial community		microbial community (clean)	text		
	339	property	334	7	day		microbial community		microbial community (clean)	text		
	340	property	334	7	day		microbial community		microbial community (clean)	text		
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	344	property	334	7	day		microbial community		microbial community (clean)	text		
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	278	property	205		48	hour	total silver		total Ag of mesocosm 3	numeric		=
	279	property	205		48	hour	total silver		total Ag of mesocosm average	numeric	#DIV/0!	=
	280	system	183		48	hour	name			text	sediment	
	281	property	280		48	hour	diameter		start of mesocosm 1	numeric		=
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	284	property	280		48	hour	diameter		start of mesocosm 2	numeric		=
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	290	property	280		48	hour	total upper Ag concentration		upper mesocosm 1 Ag concentration	numeric		=
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	293	property	280		48	hour	total upper Ag concentration		upper mesocosm average Ag concentration	numeric	#DIV/0!	=
	294	property	280		48	hour	total middle Ag concentration		middle mesocosm 1 Ag concentration	numeric		=
	295	property	280		48	hour	total middle Ag concentration		middle mesocosm 2 Ag concentration	numeric		=
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	303	property	302		48	hour	total Ag concentration		total snail Ag concentration mesocosm 1	numeric		=
	304	property	302		48	hour	total Ag concentration		total snail Ag concentration mesocosm 1	numeric		=

- **~ 5,500 overall data points**

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Conclusions – Experimental

1. Data Management is the most neglected, but highly significant experimental process
2. Can be applied from planning of experimental workflows to data analysis, preparation of research outputs and even regulatory aspects
3. Automated data curation and storage using versatile and dynamic data templates
4. Data repositories with support for tool implementation (modelling, QSARs, Omics)

Conclusions – Management

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1. Promotes data protection and security
2. Facilitates dataset QC, manipulation and analysis
3. Enhances publications and the datasets themselves are citable (DOI)
4. Can be applied from a local (single institution) to a wide (global) network to enhance harmonisation of data capture / storage
5. Significant decrease in working hours and subsequent cost
6. FAIR data and can be made Open also on demand

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Thank you

Please take our survey and let us know the tools the nanosafety community needs:

https://www.surveymonkey.co.uk/r/PK2KXWW

Contact:
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