



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



This project has received funding from the European Union Horizon 2020 Programme (H2020) under grant agreement no. 731032



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

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University of Birmingham, UK**

**OpenTox Asia 2018  
May 2018**

- 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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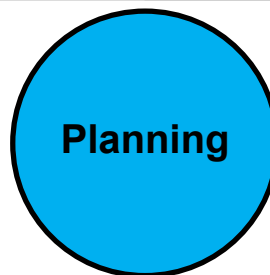
## Definition

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

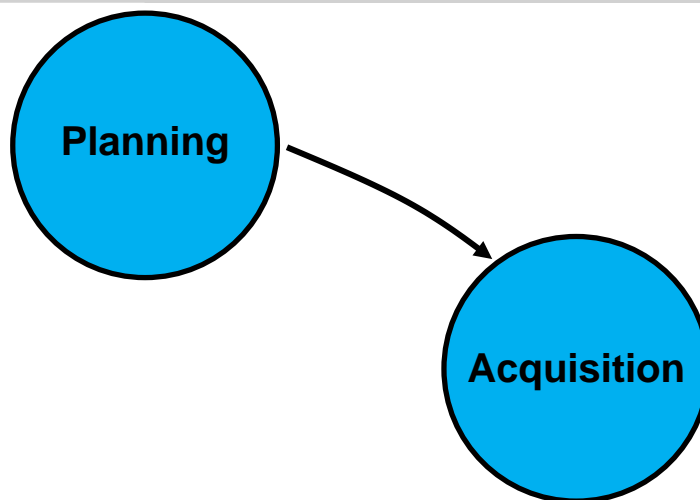
\*FAIR: Findable, Accessible, Interoperable, and Re-usable



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

# Data Lifecycle

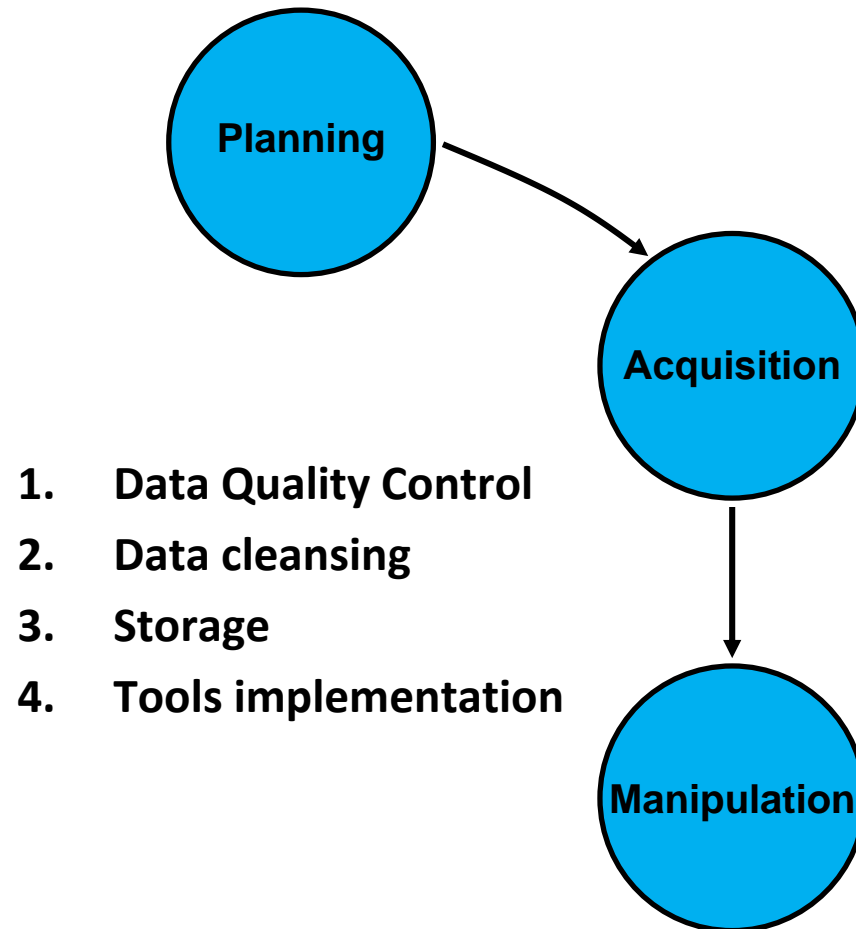
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1. Data acquisition
2. Data curation
3. Data digitisation

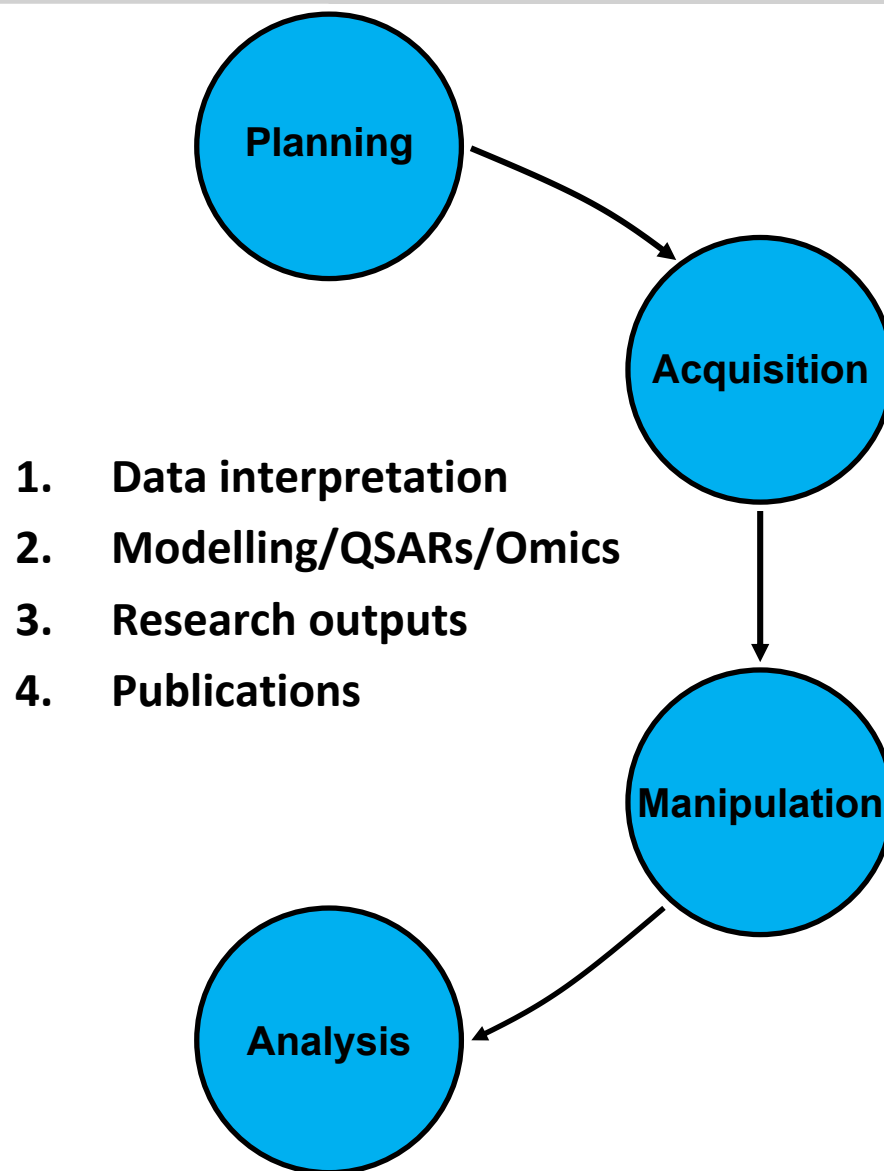
# Data Lifecycle

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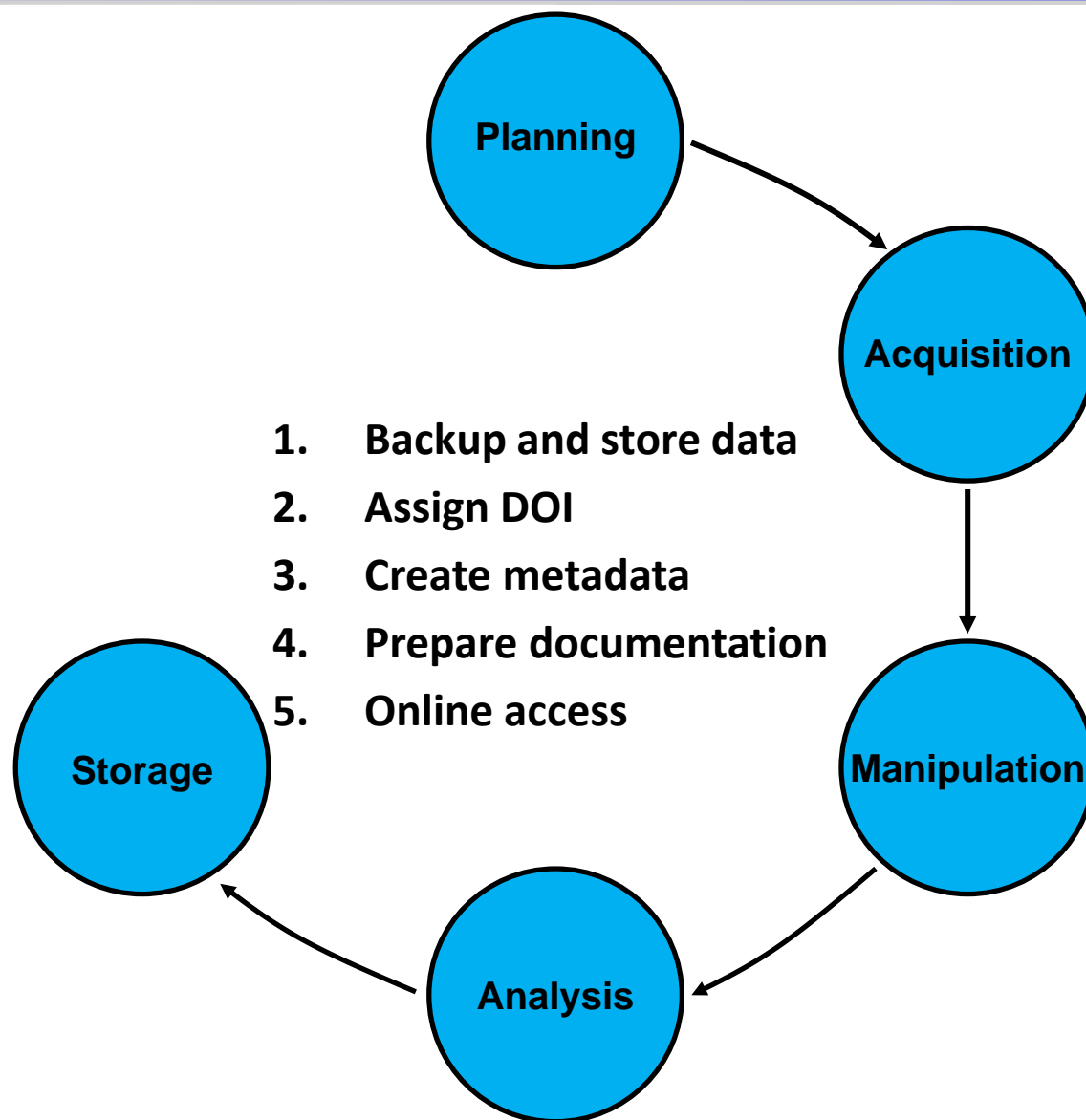
# Data Lifecycle

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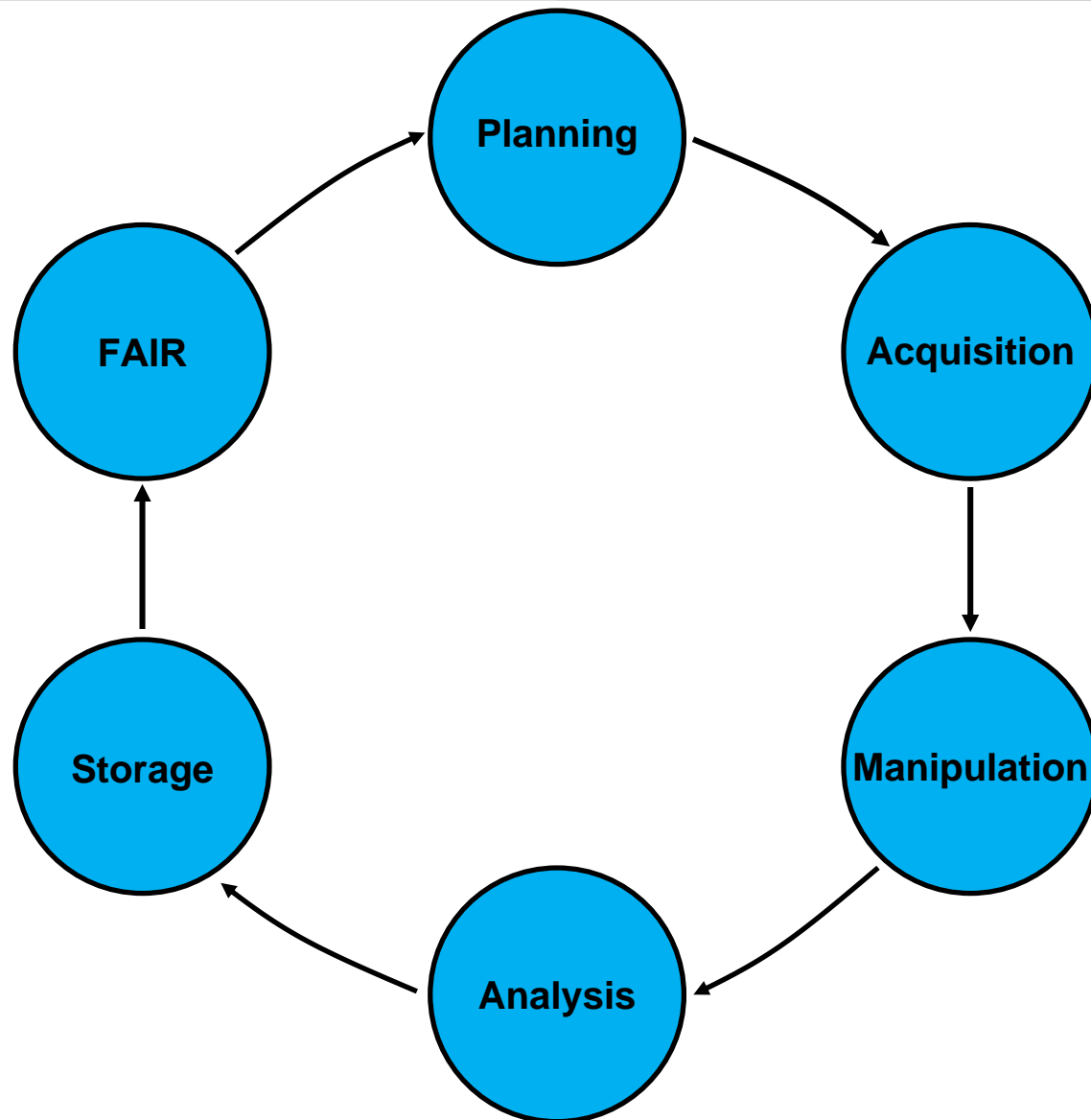


# Data Lifecycle



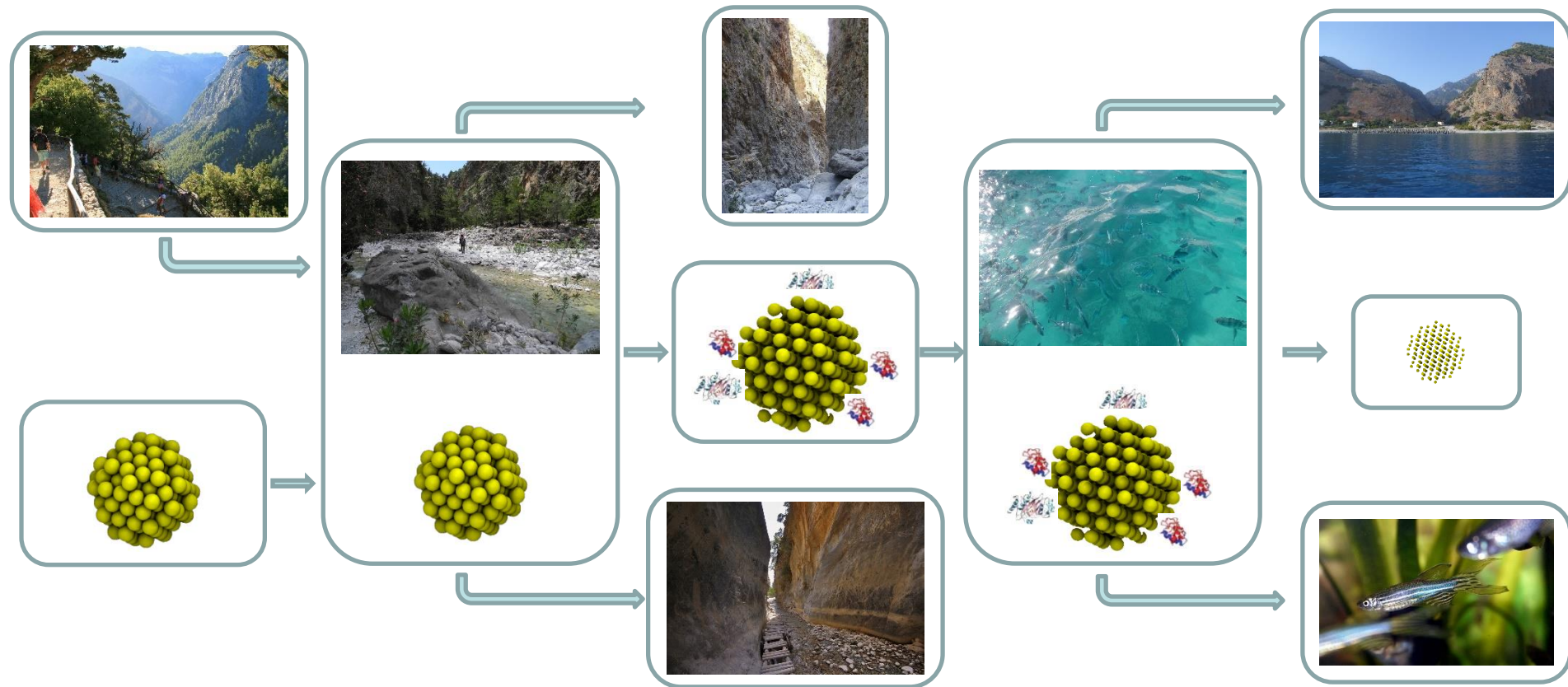
# Data Lifecycle

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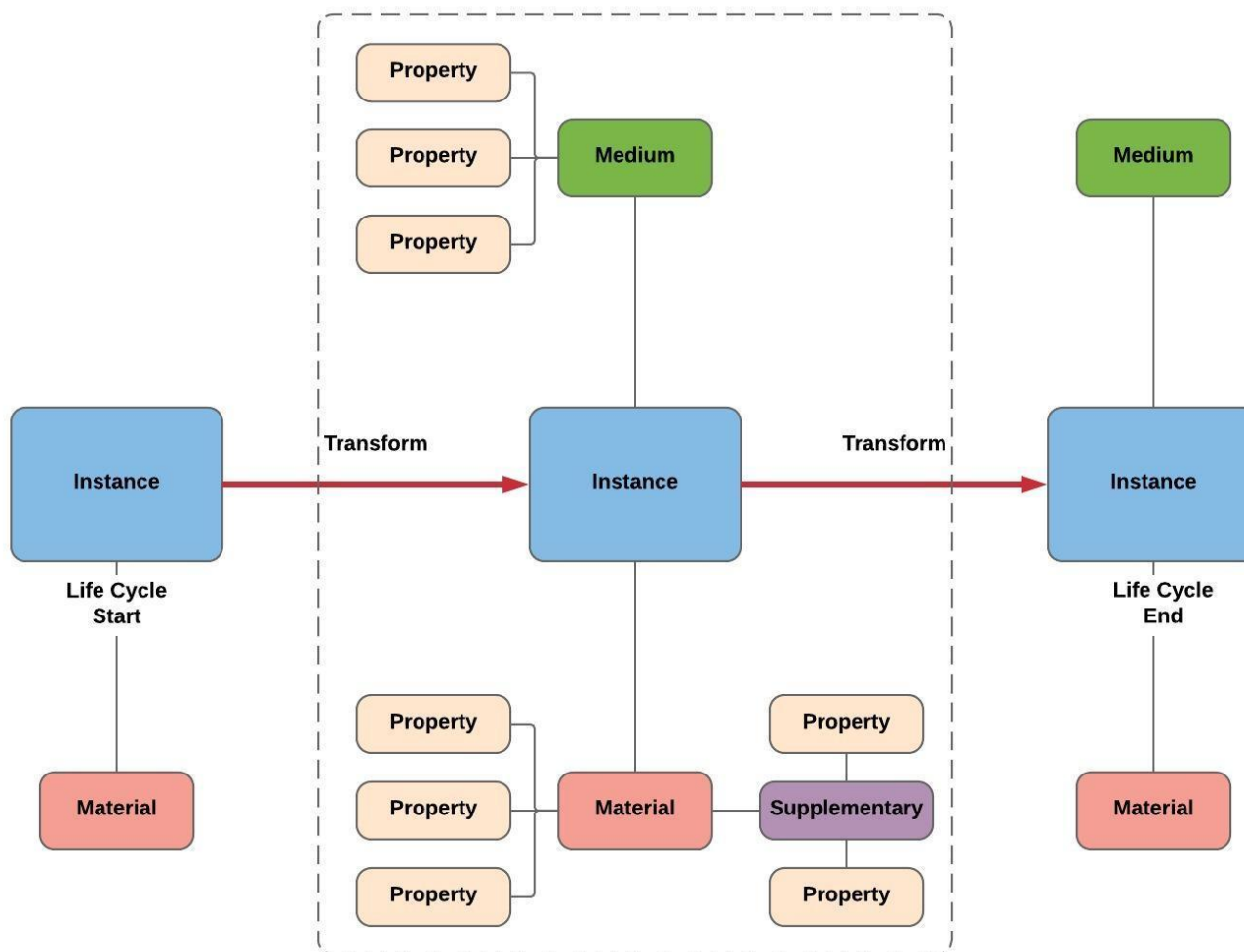
1. Data Management and Data Lifecycle
- 2. Data Curation**
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# Exposure Case Study



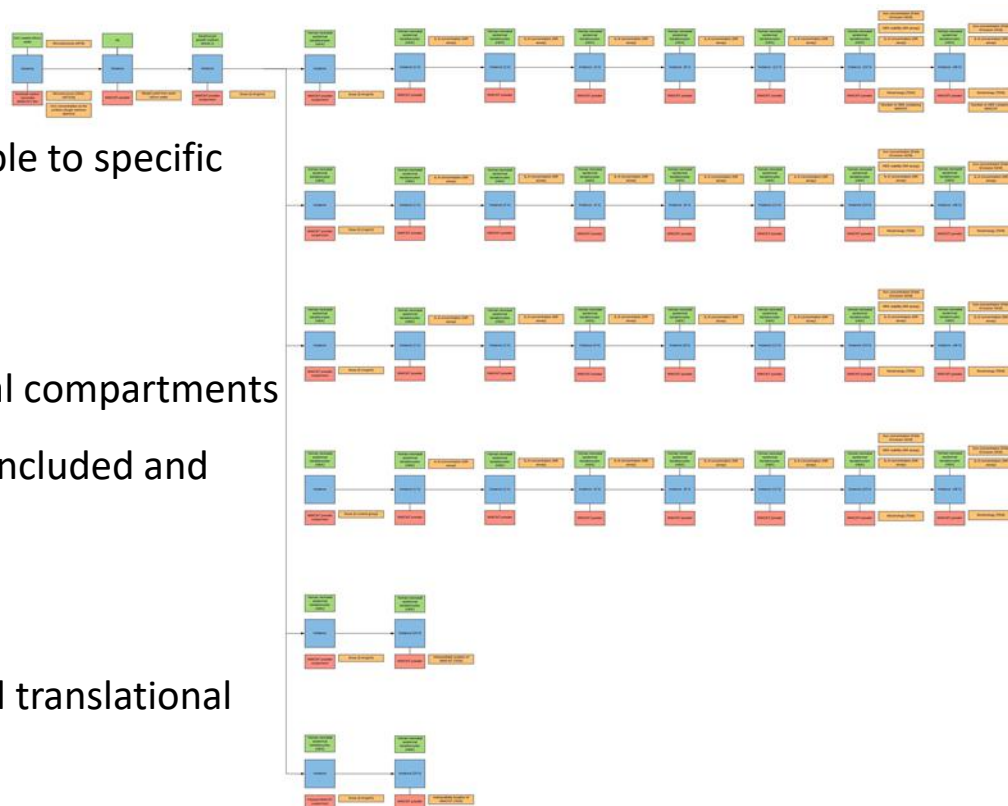
- A released nanomaterial will change itself and affect its surrounding environment

# Data Curation & NIKC Instance



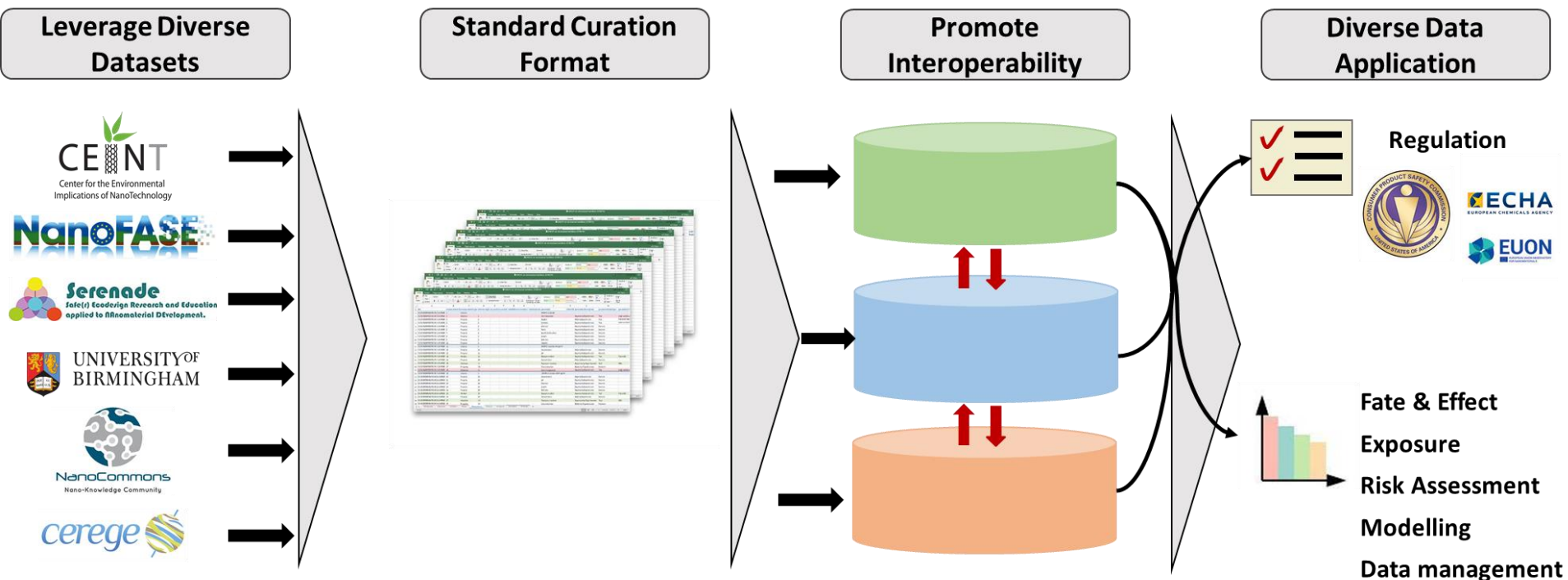
**Data Curation: The process of data collection and organisation**

# 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

1. Data Management and Data Lifecycle
2. Data Curation
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# Experimental Workflow

scinote®



NanoGroup



Hi, Anastasios Papadimitris



NanoGroup / ENM Characterisations / TiO2 Characterisation

OVERVIEW

SAMPLES

REPORTS



Edit experiment

Actions

Zoom:



+ New experiment

Stock Solution Storage Details

Due date 28.05.2018



ICP-MS Sample Preparation

Due date 29.05.2018



ICP-MS Analysis

Due date 29.05.2018



TEM Sample Preparation

Due date 28.05.2018



Average Size, Size Distribution i...

Due date 05.06.2018



Geometric Surface Area and Co...

Due date 08.06.2018



DLS Sample Preparation

Due date 28.05.2018



Hydrodynamic Diameter and PDI

Due date 29.05.2018



Zeta Potential and Electrophore...

Due date 29.05.2018



UV-VIS Sample Preparation

Due date 28.05.2018



Maximum Absorption, Wavelen...

Due date 29.05.2018








Energy Band Gap (Tauc Plots)





Due date 08.06.2018



- Multiple-branch experimental workflows

# Data Acquisition & Management

NanoGroup



Hi, Anastasios Papadiamantis


NAVIGATION

Demo for away day

- ▶ Andy's Experiment
- ▶ TIO2 Characterisation
  - ▶ TEM Characterisation
  - ▶ **DLS Characterisation**



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

PROTOCOLS RESULTS ACTIVITY **SAMPLES** REPORTS REPOSITORIES

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

Types and groups Columns


Show 10 entries Edit Delete Assign Unassign Search:





<input type="checkbox"/>	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 Papadiamantis

Showing 1 to 1 of 1 entries (0 entries selected)
Previous **1** Next




- Sample insertion and assignment

# Data Acquisition & Management


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NanoGroup / Demo for away day

/ TiO2 Characterisation / DLS Characterisation

PROTOCOLS


RESULTS

ACTIVITY

SAMPLES

REPORTS

REPOSITORIES



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>





- Fully linked analytical protocols

# Data Acquisition & Management


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/ [TiO2 Characterisation](#) / [DLS Characterisation](#)

PROTOCOLS


RESULTS


ACTIVITY


SAMPLES


REPORTS


REPOSITORIES


Add new result:


Text

Table



File

Collapse all

Expand all



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



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

**Comments**

No comments!






Your Message





+

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

- Specific experimental results

# Data Acquisition & Management

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NAVIGATION

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  - ▶ TEM Characterisation
  - ▶ **DLS Characterisation**

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/ TIO2 Characterisation / DLS Characterisation

PROTOCOLS RESULTS ACTIVITY SAMPLES REPORTS **REPOSITORIES**

Show 10 entries
Assign Unassign
Search:

<input type="checkbox"/>	Assigned	Name	measurementId	measurementType	referencingId	sourceDoi	sourceId	timeRelative	timeUnit
<input type="checkbox"/>	<input checked="" type="radio"/>	Zeta potential	07	property	5	0	0	0	0
<input type="checkbox"/>	<input checked="" type="radio"/>	Zeta potential	18	property	5	0	0	0	0
<input type="checkbox"/>	<input checked="" type="radio"/>	Temperature	30	property	17	0	0	0	0
<input type="checkbox"/>	<input checked="" type="radio"/>	Surface area	12	property	10	0	0	0	0
<input type="checkbox"/>	<input checked="" type="radio"/>	Surface area	13	property	11	0	0	0	0
<input type="checkbox"/>	<input checked="" type="radio"/>	Surface area	23	property	10	0	0	0	0
<input type="checkbox"/>	<input checked="" type="radio"/>	Surface area	24	property	11	0	0	0	0
<input type="checkbox"/>	<input checked="" type="radio"/>	Shape	25	property	12	0	0	0	0
<input type="checkbox"/>	<input checked="" type="radio"/>	Shape	14	property	12	0	0	0	0

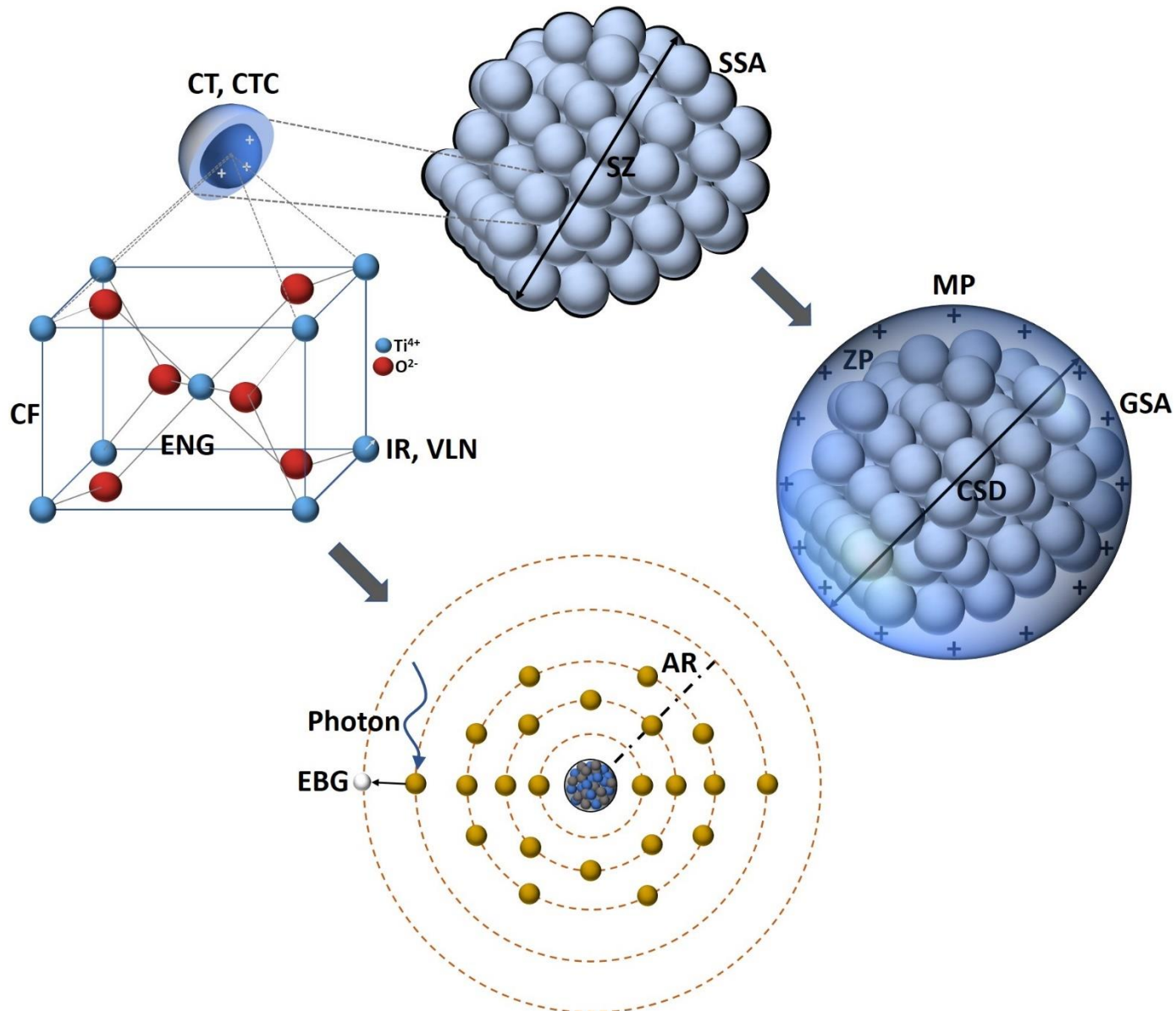
Previous
1
2
3
Next

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

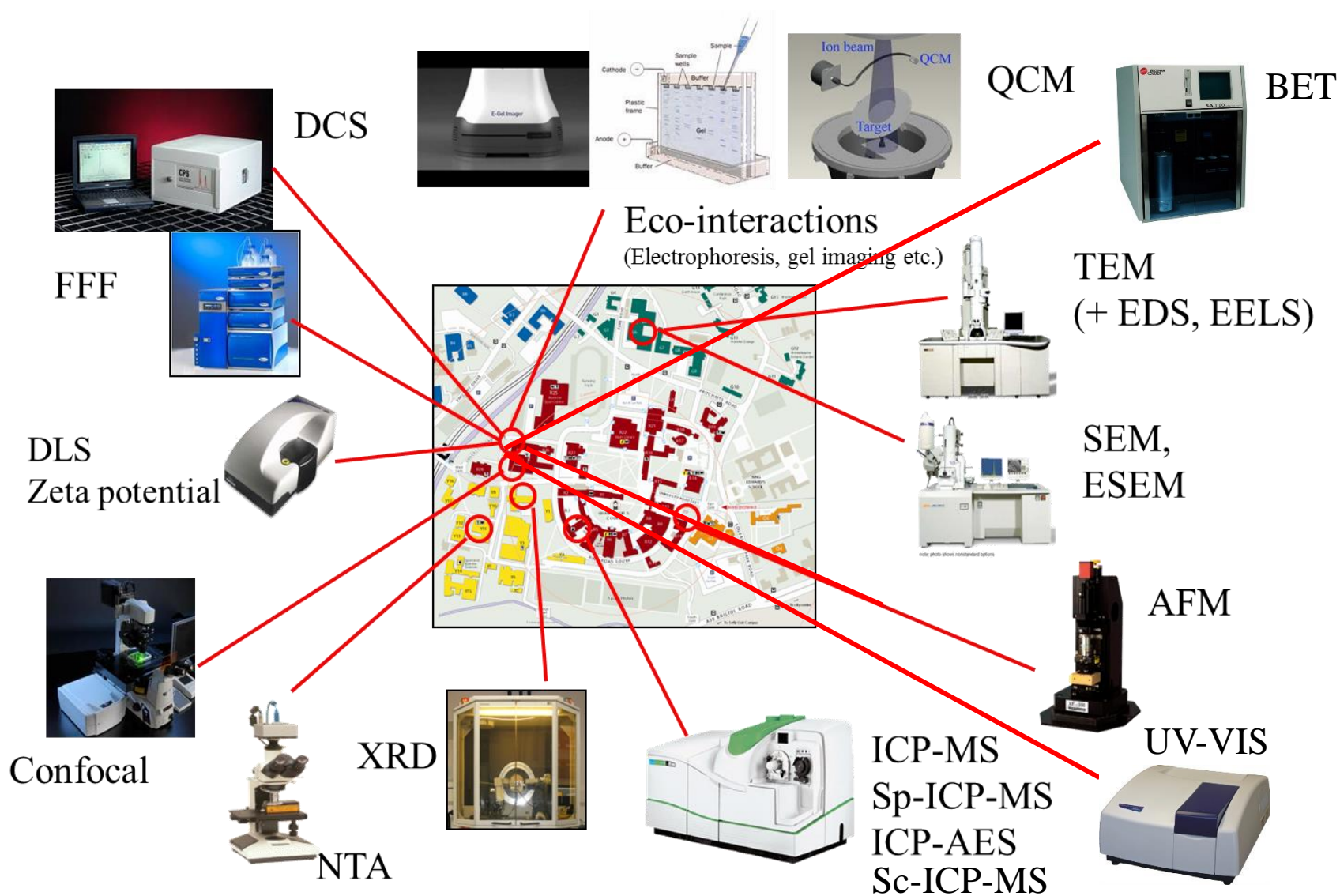
1. Data Management and Data Lifecycle
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# Nanomaterials Characterisation



# From a Local Network...





# From a Local Network...

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

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



# To a Wide Network...

ID	measurementId	measurementType	referencingId	timeRelative	timeUnit	timeAbsolute	parameter	inheritId	parameterDescription	parameterDataType	parameterText	parameter
323	property	25	7	day			Kda Ag		Kda Ag 51	numeric		
324	property	25	7	day			Kda Ag		Kda Ag 52	numeric		
325	property	25	7	day			Kda Ag		Kda Ag 53	numeric		
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		
341	property	334	7	day			microbial community		microbial community (clean)	text		
342	property	334	7	day			microbial community		microbial community (clean)	text		
343	property	334	7	day			microbial community		microbial community (clean)	text		
344	property	334	7	day			microbial community		microbial community (clean)	text		
345	property	334	7	day			microbial community		microbial community (clean)	text		
346	property	334	7	day			microbial community		microbial community (clean)	text		
347	property	334	7	day			microbial community		microbial community (clean)	text		
348	property	334	7	day			microbial community		microbial community (clean)	text		
277	property	205	48	hour			total silver		total Ag of mesocosm 2	numeric		=
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		=
282	property	280	48	hour			diameter		end of mesocosm 1	numeric		=
283	property	280	48	hour			diameter		average of mesocosm 1	numeric	#DIV/0!	=
284	property	280	48	hour			diameter		start of mesocosm 2	numeric		=
285	property	280	48	hour			diameter		end of mesocosm 2	numeric		=
286	property	280	48	hour			diameter		average of mesocosm 2	numeric	#DIV/0!	=
287	property	280	48	hour			diameter		start of mesocosm 3	numeric		=
288	property	280	48	hour			diameter		end of mesocosm 3	numeric		=
289	property	280	48	hour			diameter		average of mesocosm 3	numeric	#DIV/0!	=
290	property	280	48	hour			total upper Ag concentration		upper mesocosm 1 Ag concentration	numeric		=
291	property	280	48	hour			total upper Ag concentration		upper mesocosm 2 Ag concentration	numeric		=
292	property	280	48	hour			total upper Ag concentration		upper mesocosm 3 Ag concentration	numeric		=
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		=
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296	property	280	48	hour			total middle Ag concentration		middle mesocosm 3 Ag concentration	numeric		=
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300	property	280	48	hour			total lower Ag concentration		lower mesocosm 3 Ag concentration	numeric		=
301	property	280	48	hour			total lower Ag concentration		lower mesocosm average Ag concentration	numeric	#DIV/0!	=
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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

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

# Conclusions – Experimental

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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**



NanoCommons

Nano-Knowledge Community

***Thank you***

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

**<https://www.surveymonkey.co.uk/r/PK2KXWW>**



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