



Iseult Lynch, UoB

***Online Jaqpot Hackathon -
Take your research from the bench to the community by making your models
available as a web service***

Electronic Laboratory Notebooks

NanoCommons Workshop, 2020-06-03, #nanocommons

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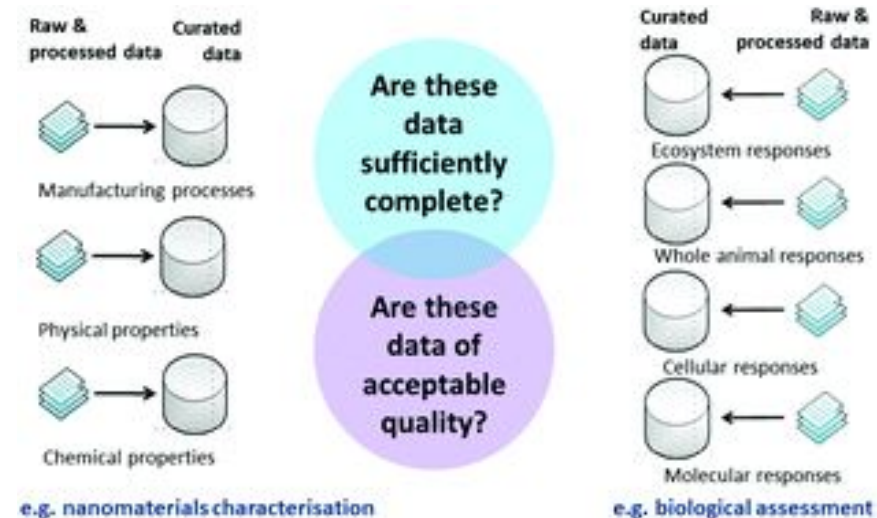
Data Management – what & why?

Definition

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

Cause & Effect

- Is the most neglected scientific process
- Most labs, at a global scale, are yet to enter the 21st century
- Poor data management can:
 - lead to significant loss of data and metadata
 - decrease the quality of data and scientific publications
 - lead to the loss of significant insights
 - Does not allow further data exploitation (e.g. AI, machine learning)

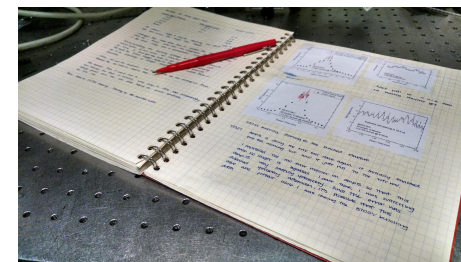


What is an Electronic Lab Notebook?

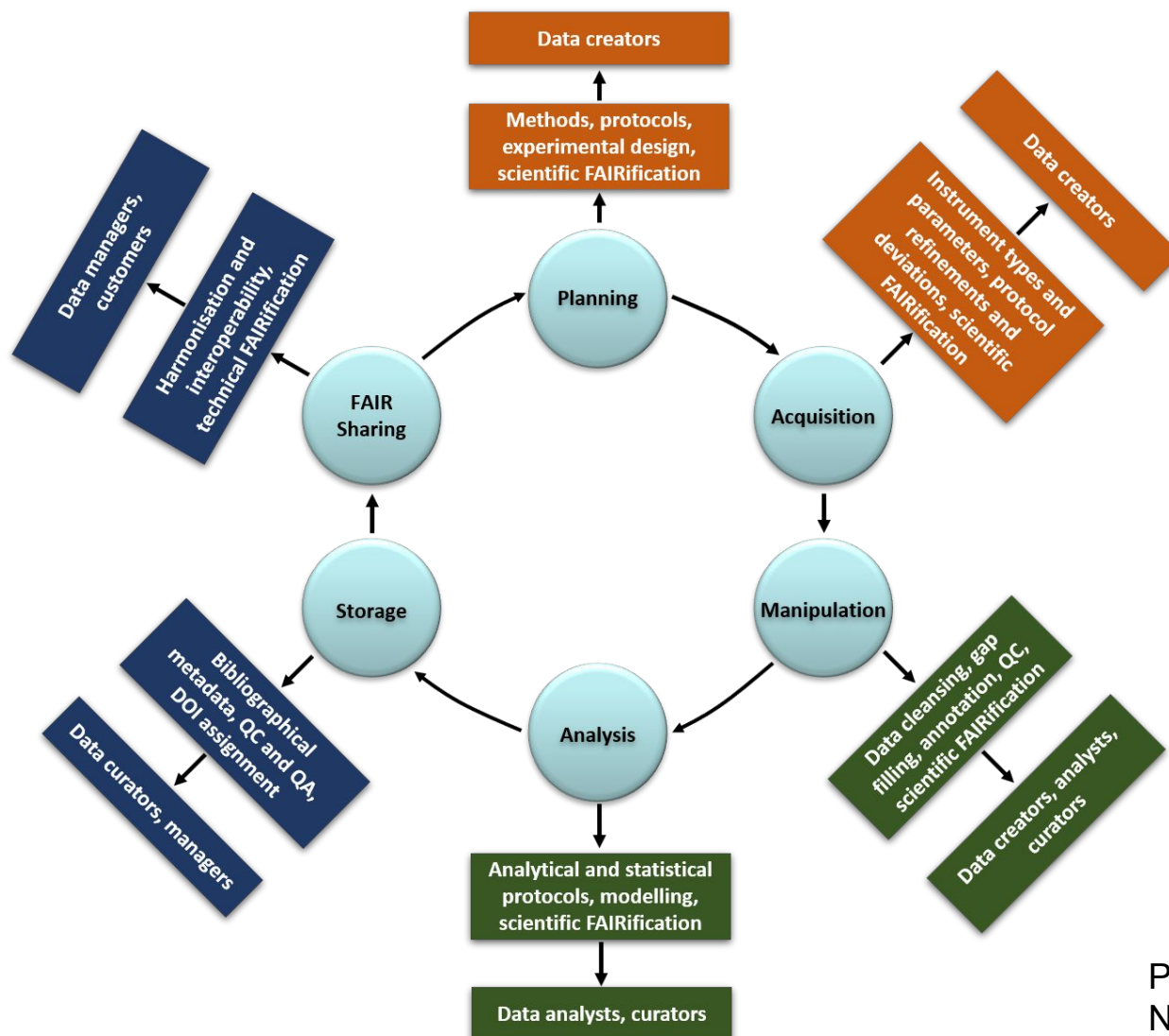
- A computer program designed to replace paper lab notebooks
- Used to manage scientific workflows, covering entire **data lifecycle**
- It can store both **data** and **metadata** information
- Lab notebooks are treated as legal documents (e.g., for patenting)!

Advantages of ELNs over PLNs:

- Easier to search within (for data, protocols, calibrations, chemicals etc.)
- Simplify data copying and backups
- Support collaboration amongst many users



Data lifecycle & metadata



Metadata is "data about data."

Descriptive metadata – assay type, cell line used, concentrations, calibrations, instrument and software parameters, etc.

Technical metadata – statistical approach, data cleaning / gap filling approach etc.

Bibliographic metadata – who generated the data, publication information, licence information, etc.

Paper for submission to Nanomaterials special issue "From Nanoinformatics to Nanomaterials Risk Assessment and Governance"

Data Management Plan

1. Data Collection and Documentation

☐

☐ What kind of data are generated

☐ How will data be generated

☐ What metadata are needed

2. Ethics, legal and security Issues

☐

☐ How will ethical issues be handled

☐ How are the data accessed

☐ Are there copyright issues

☐ Are there sensitive data

☐ What about intellectual property rights

3. Data Storage and Preservation

☐

☐ How are the data stored?

☐ Are there back up systems

☐ How are data safely preserved

4. Data Sharing and reuse

☐

☐ How and where will the data be shared?

☐ How are sensitive data protected

☐ How can data be accessed

<https://www.nanocommons.eu/deliverable-d10-1-v2-0-second-version-of-nanocommons-data-management-plan/>

Please feel free to use it / built on it. V3.0 coming shortly with more specific examples of managing access to specific datasets – experimental, computational and literature curated.

Multiple ELN suppliers

https://labsexplorer.s3-eu-west-1.amazonaws.com/content/files/list-eln-summary_40e11eff-1584348490.pdf

	Intend for...	Highlighted features	Format	Pricing	Score
Labfolder	All scientific fields	Timestamps Digital signature	SaaS, software	Free for 3 users 3+ paid users	24
LabArchives	All scientific fields	Integration with LIMS Features modules	SaaS + Apps	Free plan Paid plan	22
sciNote	All scientific fields	Export all data Integration with other softwares	SaaS Software	Free plan Premium plan	21
eLabFTW	All scientific fields	Timestamps Integration with some lab tools	Open-sour ce software	Free	21
Benchling	Biology Chemistry	Timestamps Free for academics	SaaS	Free plan Paid plan	20
eLabJournal	Life science	App available Workflow management	SaaS Mobile app	From 10€/month/user	20
Labii ELN	All scientific fields	Integration with LIMS Pay per use	SaaS	Pay-as-you-go plan	20
Findings	All scientific fields	Progress tracker Quick access to resources	iOs	Free plan Paid plan	20
Uncountable	Chemistry engineering fields	AI-based suggestions for experiments	SaaS	Price on request	19
RSpace	All scientific fields	Data encryption Intuitive design	SaaS Software	Free plan Premium plan	19
Hivebench	Life science	Electronic signature Automatic backups	SaaS Software	Free plan Premium plan	19

Ranked according to following criteria:

User-friendliness: 0-5 points

Completeness: 0-5 points

Connectivity (to equipment / other
software): 0-5 points

Price: 0 to 5 points

Special bonus points are given by Labs
Explorer's team members up to 5.



[illegible]

The screenshot shows the SCIONet application interface. At the top, there's a navigation bar with the SCIONet logo and user information. Below it, a sidebar on the left contains navigation links: 'New for easy day', 'Easy Characterization', 'New Characterization', 'Filter Characterization', and 'Old Characterization'. The main content area is titled 'New for easy day' and 'New Characterization'. It features a table with the following columns: ID, Name, Type, Location, and Status. The table contains several rows of data, including 'Data potential', 'Temperature', 'Surface area', and 'Ships'. At the bottom right, there are buttons for 'Previous' and 'Next'.

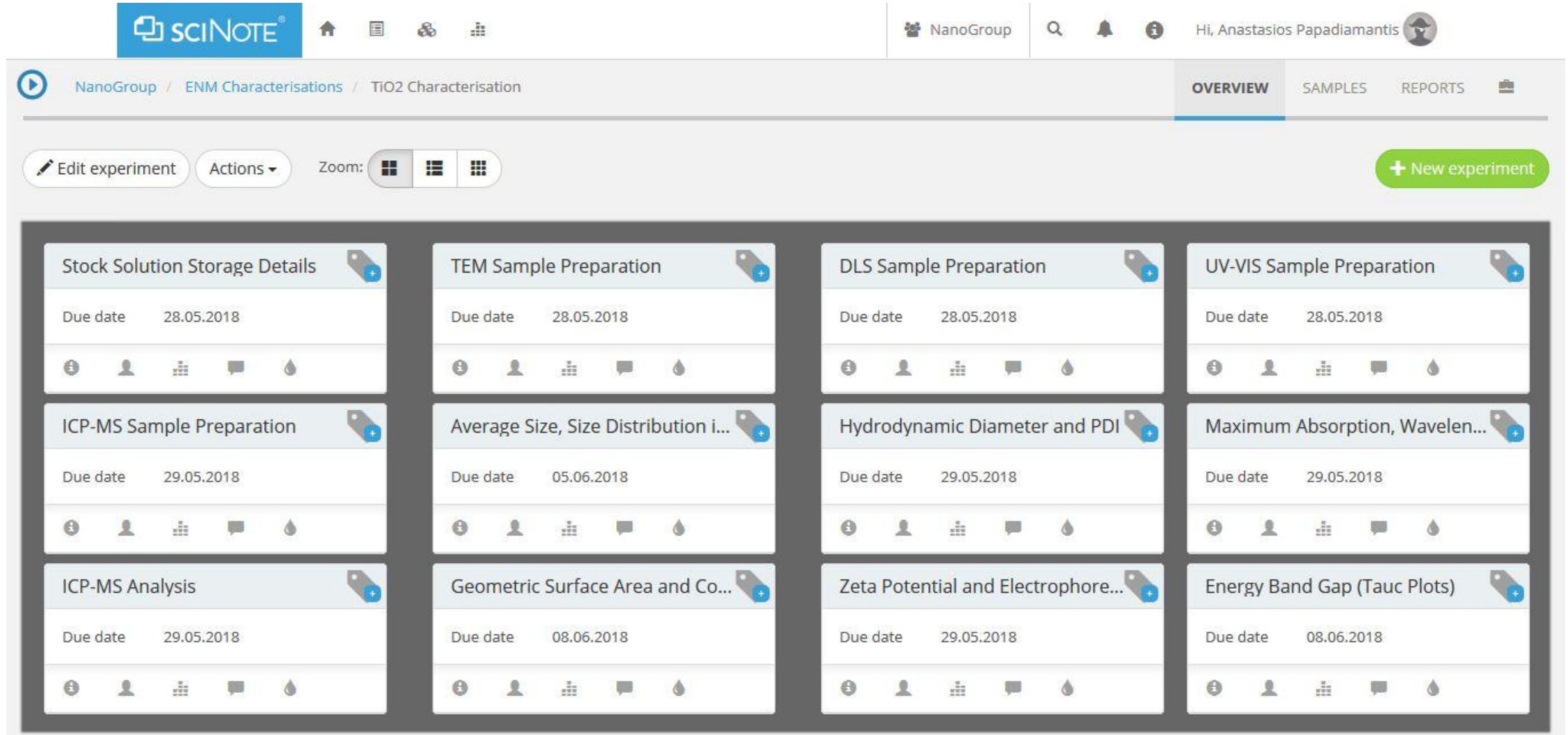
ID	Name	Type	Location	Status
1	Data potential	property	5	0
2	Data potential	property	5	0
3	Temperature	property	17	0
4	Surface area	property	10	0
5	Surface area	property	11	0
6	Surface area	property	10	0
7	Surface area	property	11	0
8	Ships	property	12	0
9	Ships	property	11	0

The screenshot displays the SciNote application interface. At the top, the SciNote logo is on the left, and navigation icons (home, search, user profile) are on the right. Below the logo, the 'NAVIGATION' sidebar on the left contains links for 'Home for easy life', 'Add new Experiment', 'ECG Characterization', and 'ECG Characterization' (selected). The main content area shows a header with 'NewExperiment - Sample for easy life', 'ECG Characterization', and 'ECG Characterization'. Below this, there are tabs for 'PROTOCOLS', 'RESULTS', 'ACTIVITY', and 'SAMPLES' (selected). The 'SAMPLES' tab displays a table of samples. The table has columns for 'Types and groups' and 'Columns'. The table content includes a row with 'Accepted', 'Sample name', 'Sample type', 'Sample group', 'Add on', and 'Add by'. The 'Sample name' column shows 'T02 (ECG 140101)', 'ECG Apnea Solution', and 'ECG ECG-Rhythm'. The 'Sample type' column shows 'ECG Apnea Solution', 'ECG ECG-Rhythm', and 'ECG ECG-Rhythm'. The 'Sample group' column shows 'ECG Apnea Solution', 'ECG ECG-Rhythm', and 'ECG ECG-Rhythm'. The 'Add on' column shows '15.02.2018 02:14' and '15.02.2018 02:14'. The 'Add by' column shows 'Andreas Papadimitriou'. Below the table, it says 'Showing 1 to 1 of 1 entries (0 entries selected)'. At the bottom right, there is a 'Previous' button and a 'Next' button.

[illegible]

The screenshot displays the SciNote application interface. At the top, there is a navigation bar with the SciNote logo, a search bar, and a user profile icon. Below the navigation bar, there is a breadcrumb trail showing 'Homegroup' and 'TGS Characterization'. The main content area is a dashboard with a grid of analysis modules. Each module has a title, a 'Due date' (all set to 20/05/2018), and a status bar with icons for 'View', 'Edit', 'Share', and 'Delete'. The modules include: 'Stock Solution Storage Details', 'TSM Sample Preparation', 'DLS Sample Preparation', 'UV-Vis Sample Preparation', 'ICP-MS Sample Preparation', 'Average Size, Size Distribution L...', 'Hydrodynamic Diameter and PDI', 'Maximum Absorption, Wavelength', 'ICP-MS Analysis', 'Geometric Surface Area and Co...', 'Zeta Potential and Electrophore...', and 'Energy Band Gap (Eg, Pn)'. A 'New experiment' button is located in the top right corner of the dashboard area.

Data capture: Experimental Workflow



The screenshot displays the SciNote web application interface for managing experimental workflows. At the top, the SciNote logo is on the left, and user information (NanoGroup, search, notifications, and user profile) is on the right. The main header shows the breadcrumb path: NanoGroup / ENM Characterisations / TiO2 Characterisation. Below this, there are tabs for OVERVIEW, SAMPLES, and REPORTS. A toolbar includes an 'Edit experiment' button, an 'Actions' dropdown, a 'Zoom' control with three grid icons, and a '+ New experiment' button. The main content area is a grid of 12 task cards, each representing a step in the workflow. Each card has a title, a due date, and a set of icons for information, user assignment, data visualization, communication, and a reminder. The tasks are organized into four columns and three rows.

Task Name	Due Date
Stock Solution Storage Details	28.05.2018
TEM Sample Preparation	28.05.2018
DLS Sample Preparation	28.05.2018
UV-VIS Sample Preparation	28.05.2018
ICP-MS Sample Preparation	29.05.2018
Average Size, Size Distribution i...	05.06.2018
Hydrodynamic Diameter and PDI	29.05.2018
Maximum Absorption, Wavelen...	29.05.2018
ICP-MS Analysis	29.05.2018
Geometric Surface Area and Co...	08.06.2018
Zeta Potential and Electrophore...	29.05.2018
Energy Band Gap (Tauc Plots)	08.06.2018

- Multiple-branch experimental workflows

Data Acquisition & Management

sciNOTE®

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:






	Assigned	Sample name	Sample type	Sample group	Added on	Added by
<input type="checkbox"/>	<input checked="" type="checkbox"/>	TiO2 JRC NM103	ENM Aqueous Solution	* TiO2 ENM Rutile	15.02.2018 23:14	Anastasios Papadimitantis

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





Previous 1 Next

- Sample insertion and assignment

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

PROTOCOLSRESULTSACTIVITYSAMPLESREPORTSREPOSITORIES

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







NanoGroup



Hi, Anastasios Papadiamantis



NAVIGATION



NanoGroup / Demo for away day

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 Papadiamantis



	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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NanoGroup

Hi, Anastasios Papadimitris

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

Show 10 entries ☒ Assign ☐ Unassign Search:

<input type="checkbox"/>	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
<input type="checkbox"/>	●	Surface area	24	property	11	0	0	0	0
<input type="checkbox"/>	●	Shape	25	property	12	0	0	0	0
<input type="checkbox"/>	●	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

Transnational Access – Help to set up your ELNs



**Experimental Workflows
Design & Implementation**



**Data Processing
& Analysis**



**Data Visualisation
& Predictive Toxicity**



**Data Storage
& Online Accessibility**

<https://www.nanocommons.eu/apply-for-access/>

<https://www.nanocommons.eu/contact/>

Nanomaterials characterisation

Nanomaterials bio-nano interactions: protein and metabolite coronas etc.

Nanomaterials environmental fate & transformations

Toxicity and Ecotoxicity (in vitro and in vivo) assays, including high throughput and omics approaches

Image analysis etc.



Thank you & Questions?