



NanoCommons

Nano-Knowledge Community

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



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NanoCommons

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***Electronic Lab Notebooks
Demo of NanoCommons-powered Features***

**ELN Hackathon
13 January 2022**

What are laboratory notebooks

Definition

A laboratory notebook is the main means for recording research.

Scope

- Document hypotheses
- Design experiments and experimental procedures
- Record methods/protocols
- Record experimental settings
- Record observations / data
- Initial analysis / interpretation
- Protect intellectual property

Traditional laboratory notebooks

The bottlenecks

- Paper...
- Slow recording, often post experiment, missed information
- Expensive, need huge storage space
- Cannot be backed up (realistically)
- Cannot be searched
- Difficult to decipher
- Lack of collaboration (in practice)
- Reproducibility

Traditional laboratory notebooks

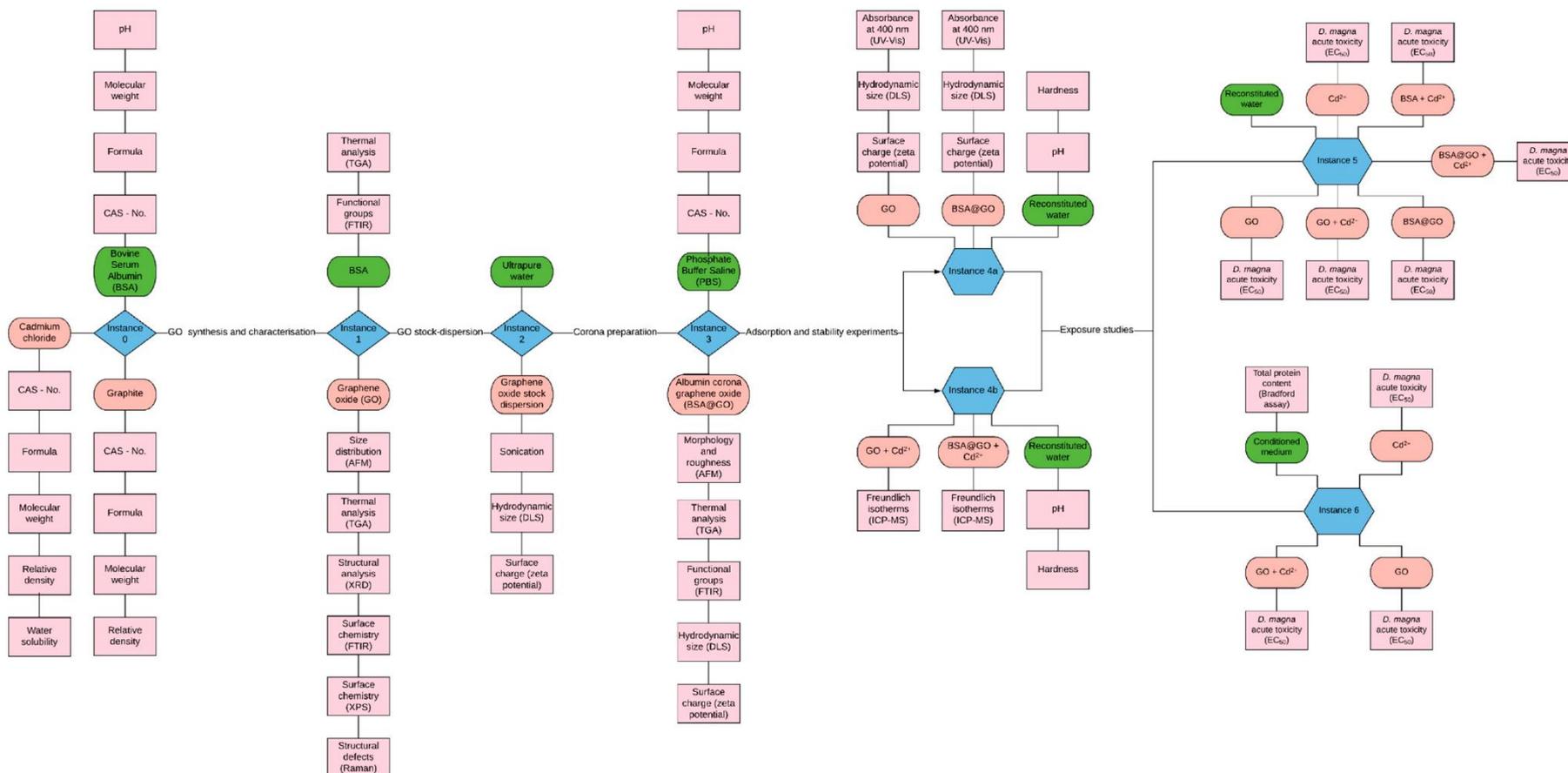
Case study – Research Laboratory

- Reproduce an experiment from 5 years ago:
 - Identify the correct lab book
 - Identify the correct experiment
 - Understand someone else's writing
 - Decode the writing method
 - Understand the process
 - Understand the settings
 - Retrieve the original raw data (where from?)
 - Do the experiment...



Traditional laboratory notebooks

Case study – Research Laboratory



Electronic laboratory notebooks

Requirements

- Team creation and sharing
- Local or cloud based (but definitely networked)
- Text input (notes, data, deviations...)
- Data import
- Import images and annotations
- Protocols repository
- Searchable
- Report creation
- APIs

Electronic laboratory notebooks

The benefits

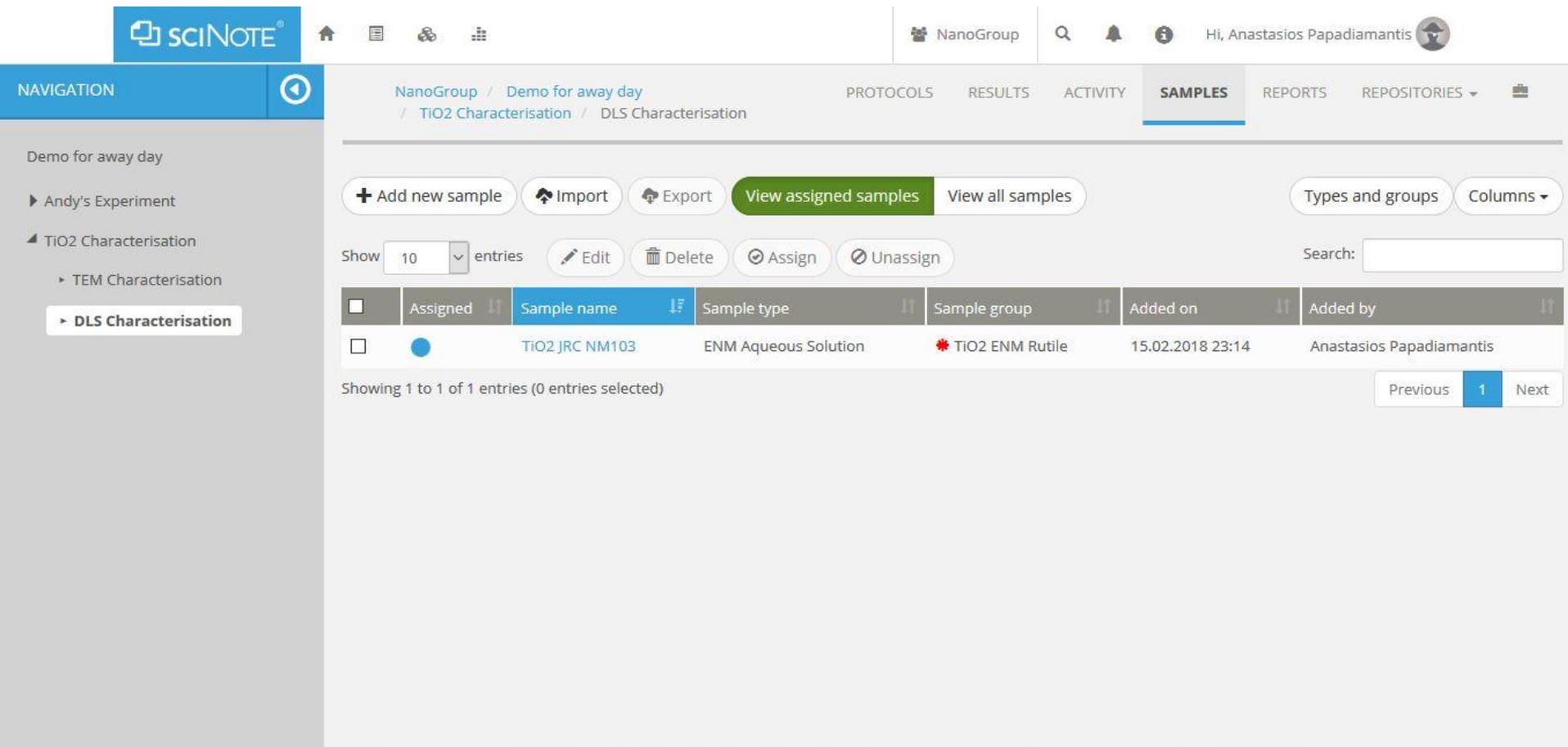
- Streamlined project management
- Local or cloud based
- Easy to setup complex experiments (compared to traditional lab books)
- Protocol method integration
- Notes / settings / deviation recording
- Quick data recording
- Direct data digitisation
- QA / QC
- Team-wide collaboration

Electronic laboratory notebooks

The barriers

- Established habits
- Lack of time
- Lack of data management literacy
- Mistrust of cloud-based / digital tools
- Heavy transition burden
- Training requirements

Data Acquisition & Management



The screenshot displays the SciNote web application interface. At the top, the SciNote logo is on the left, and the user profile 'Hi, Anastasios Papadiamantis' is on the right. The main navigation bar includes 'NanoGroup', 'PROTOCOLS', 'RESULTS', 'ACTIVITY', 'SAMPLES' (highlighted), 'REPORTS', and 'REPOSITORIES'. The breadcrumb trail shows 'NanoGroup / Demo for away day / TIO2 Characterisation / DLS Characterisation'. The left sidebar contains a 'NAVIGATION' menu with 'Demo for away day', 'Andy's Experiment', 'TIO2 Characterisation', 'TEM Characterisation', and 'DLS Characterisation' (highlighted). The main content area features a toolbar with '+ Add new sample', 'Import', 'Export', 'View assigned samples' (highlighted), and 'View all samples'. Below the toolbar, there are controls for 'Show 10 entries', 'Edit', 'Delete', 'Assign', and 'Unassign', along with a search box. A table lists sample entries with columns for 'Assigned', 'Sample name', 'Sample type', 'Sample group', 'Added on', and 'Added by'. One entry is visible: 'TIO2 JRC NM103' (ENM Aqueous Solution) assigned to 'TIO2 ENM Rutile' on '15.02.2018 23:14' by 'Anastasios Papadiamantis'. At the bottom, it shows 'Showing 1 to 1 of 1 entries (0 entries selected)' and navigation buttons 'Previous', '1', and 'Next'.

- **Sample insertion and assignment**

Data Acquisition & Management

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.

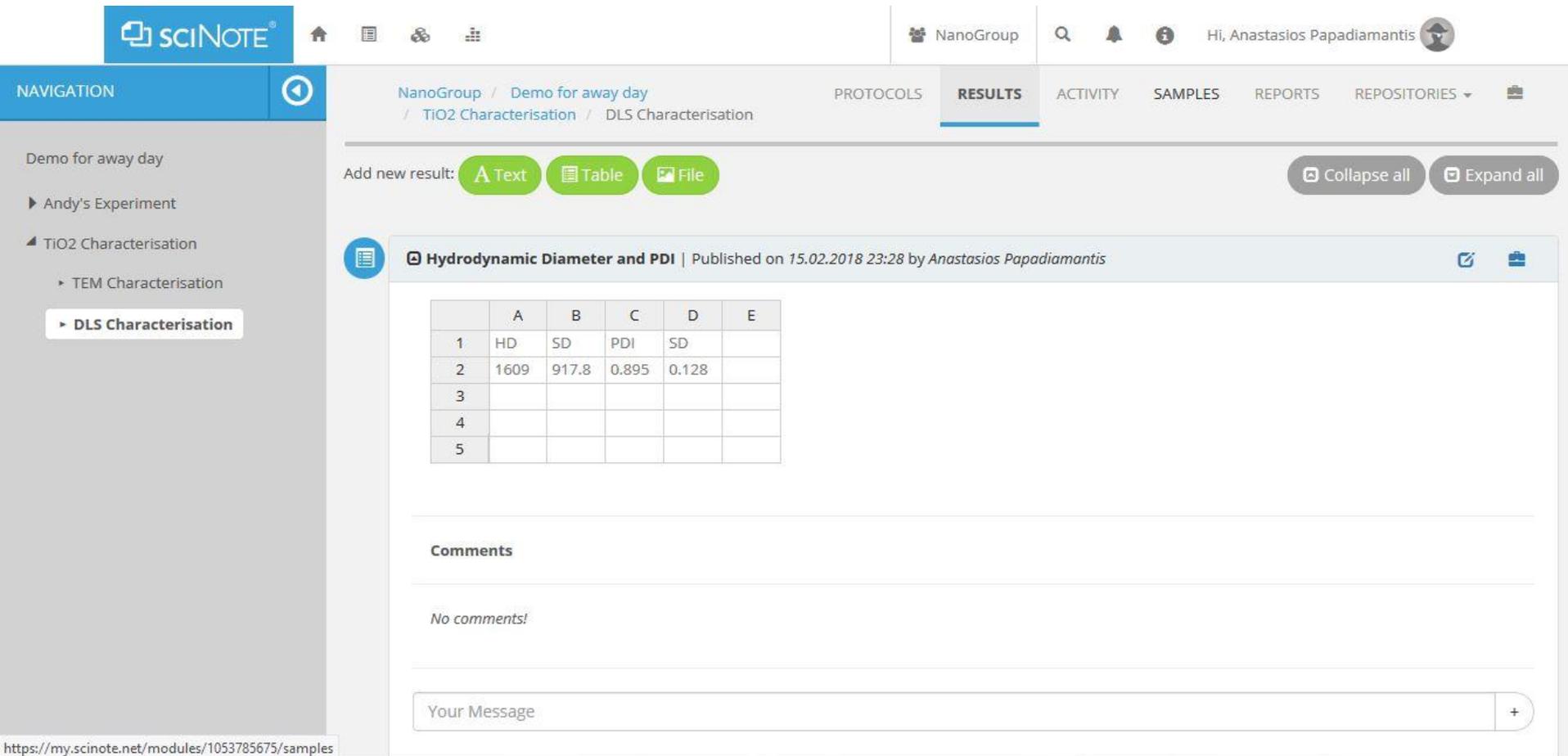
Zeta Potential – A zeta potential cuvette was injected with about 1 mL of the liquid to be analysed and was then placed in the sample holder of the Malvern Zetasizer (nano ZS). A standard operating procedure was once again set up for each material and involved inputting the refractive index and absorption 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>

- Fully linked analytical protocols

Data Acquisition & Management



The screenshot displays the SciNote web interface. At the top, the SciNote logo is on the left, and the user's name 'Hi, Anastasios Papadiamantis' is on the right. The main navigation bar includes 'NanoGroup', 'PROTOCOLS', 'RESULTS' (highlighted), 'ACTIVITY', 'SAMPLES', 'REPORTS', and 'REPOSITORIES'. Below this, the breadcrumb path is 'NanoGroup / Demo for away day / TiO2 Characterisation / DLS Characterisation'. The 'Add new result:' section offers options for 'Text', 'Table', and 'File'. The main content area shows a table titled 'Hydrodynamic Diameter and PDI' published on 15.02.2018 23:28 by Anastasios Papadiamantis. The table has 5 rows and 5 columns (A-E). The first row contains headers: HD, SD, PDI, SD. The second row contains values: 1609, 917.8, 0.895, 0.128. Below the table is a 'Comments' section with the text 'No comments!' and a 'Your Message' input field.

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 result: **Text** Table File

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

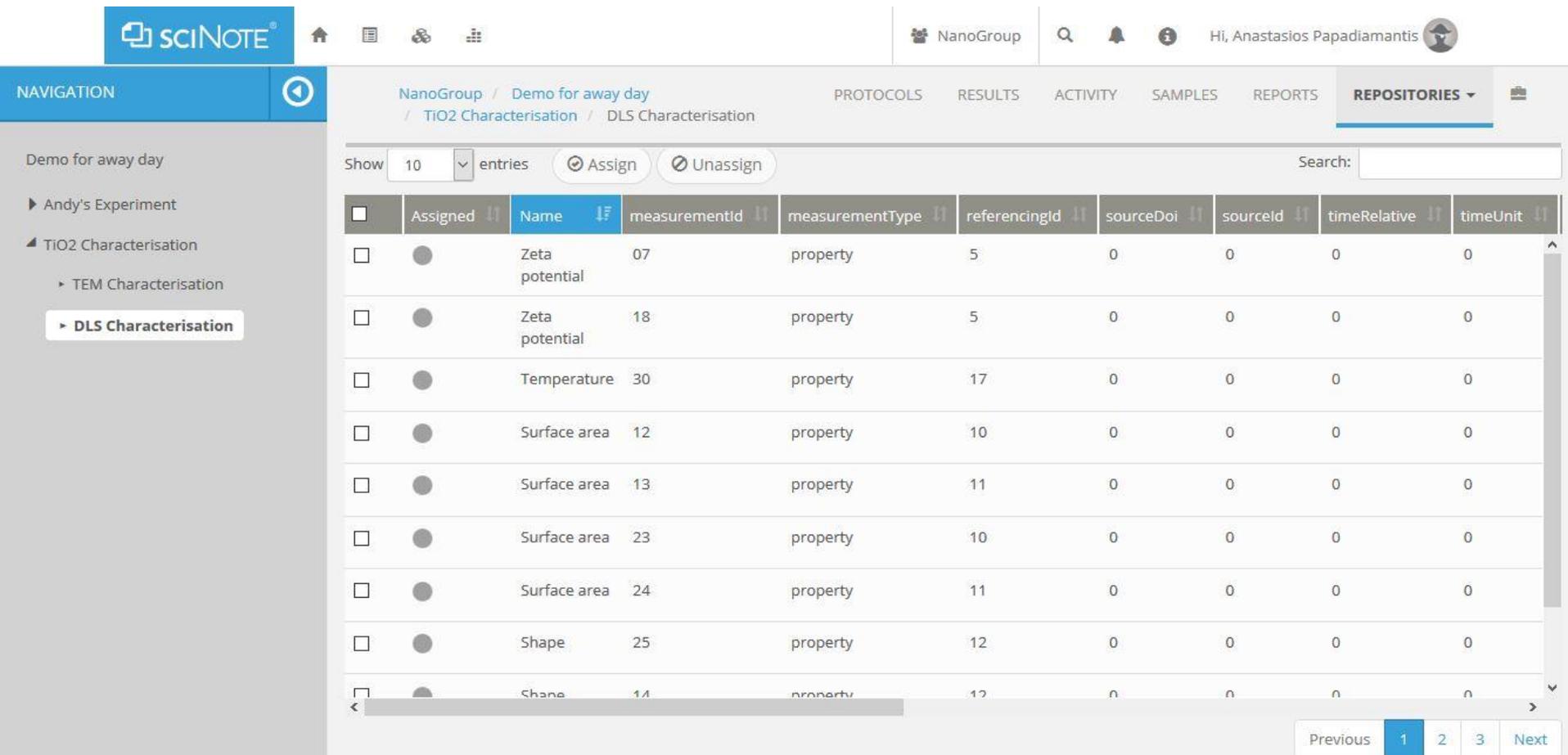
No comments!

Your Message

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

- **Specific experimental results**

Data Acquisition & Management



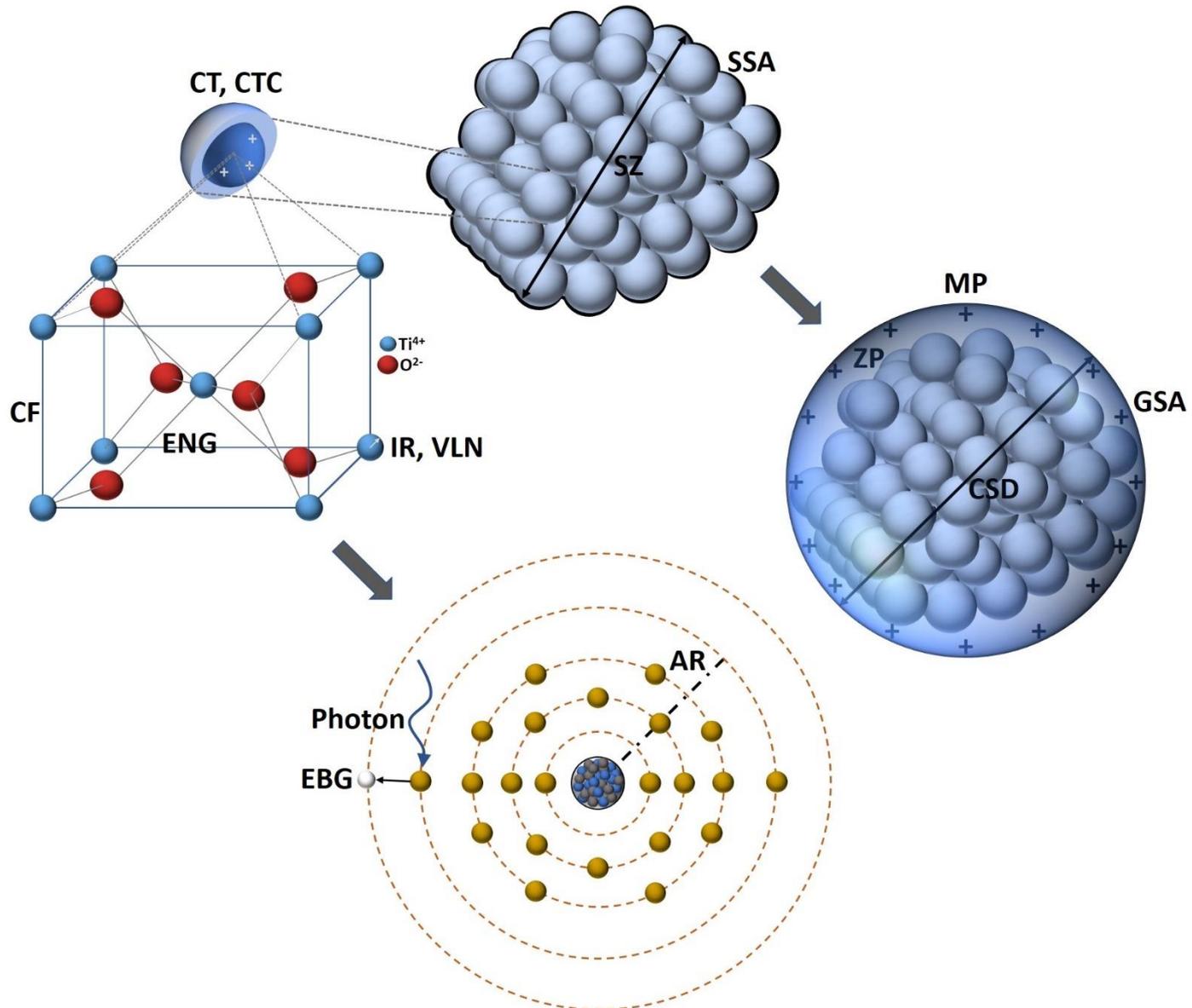
The screenshot displays the SciNote web interface. The top navigation bar includes the SciNote logo, a home icon, a calendar icon, a network icon, and a list icon. The user is logged in as 'Hi, Anastasios Papadiamantis'. The main content area shows a breadcrumb trail: 'NanoGroup / Demo for away day / TIO2 Characterisation / DLS Characterisation'. Below this, there are tabs for 'PROTOCOLS', 'RESULTS', 'ACTIVITY', 'SAMPLES', 'REPORTS', and 'REPOSITORIES'. A table of data is displayed with columns: 'Assigned', 'Name', 'measurementId', 'measurementType', 'referencingId', 'sourceDoi', 'sourceId', 'timeRelative', and 'timeUnit'. The table contains 10 rows of data. At the bottom right, there is a pagination control showing 'Previous', '1', '2', '3', and 'Next'.

<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

- Automatic extraction and shipment to data repository via email

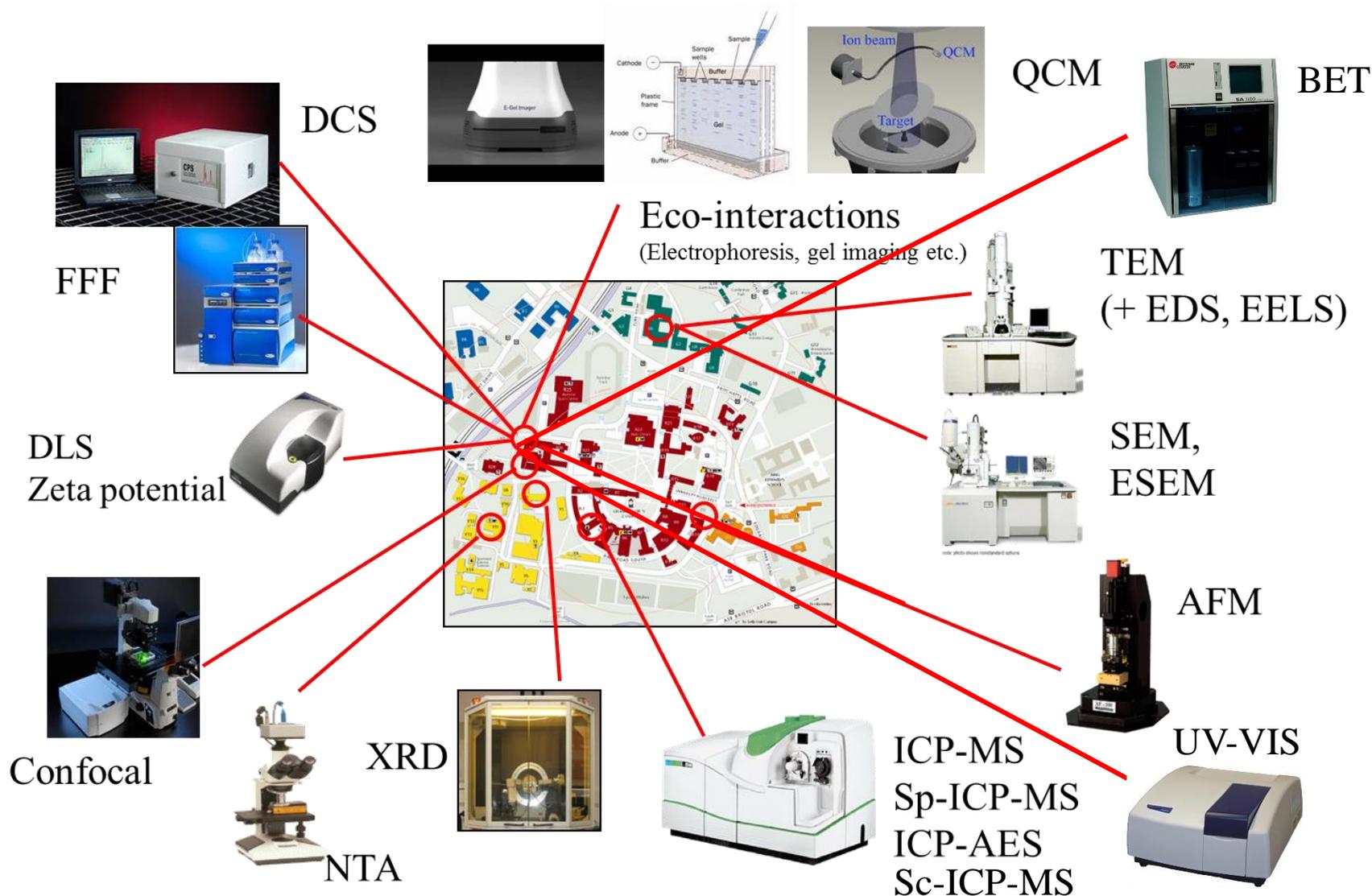
Case study

Nanomaterials Characterisation





From a Local Network...



Experimental Workflow

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

To a Wide Network...



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To a Wide Network...

Projects / ACEnano Inter Laboratory Com... /

UV-VIS Inter Laboratory Comparison

Edit Experiment

Actions ▾

Zoom:



BfR UV-Vis Round Robin

Completed on 08/29/2018

Completed



KRISS UV-Vis Round Robin

Completed on 07/25/2018

Completed



NERC UV-Vis Round Robin

Completed on 09/03/2018

Completed



UFZ UV-Vis Round Robin

Completed on 09/03/2018

Completed



UoB UV-Vis Round Robin

Completed on 09/04/2018

Completed



UoOxf Round Robin

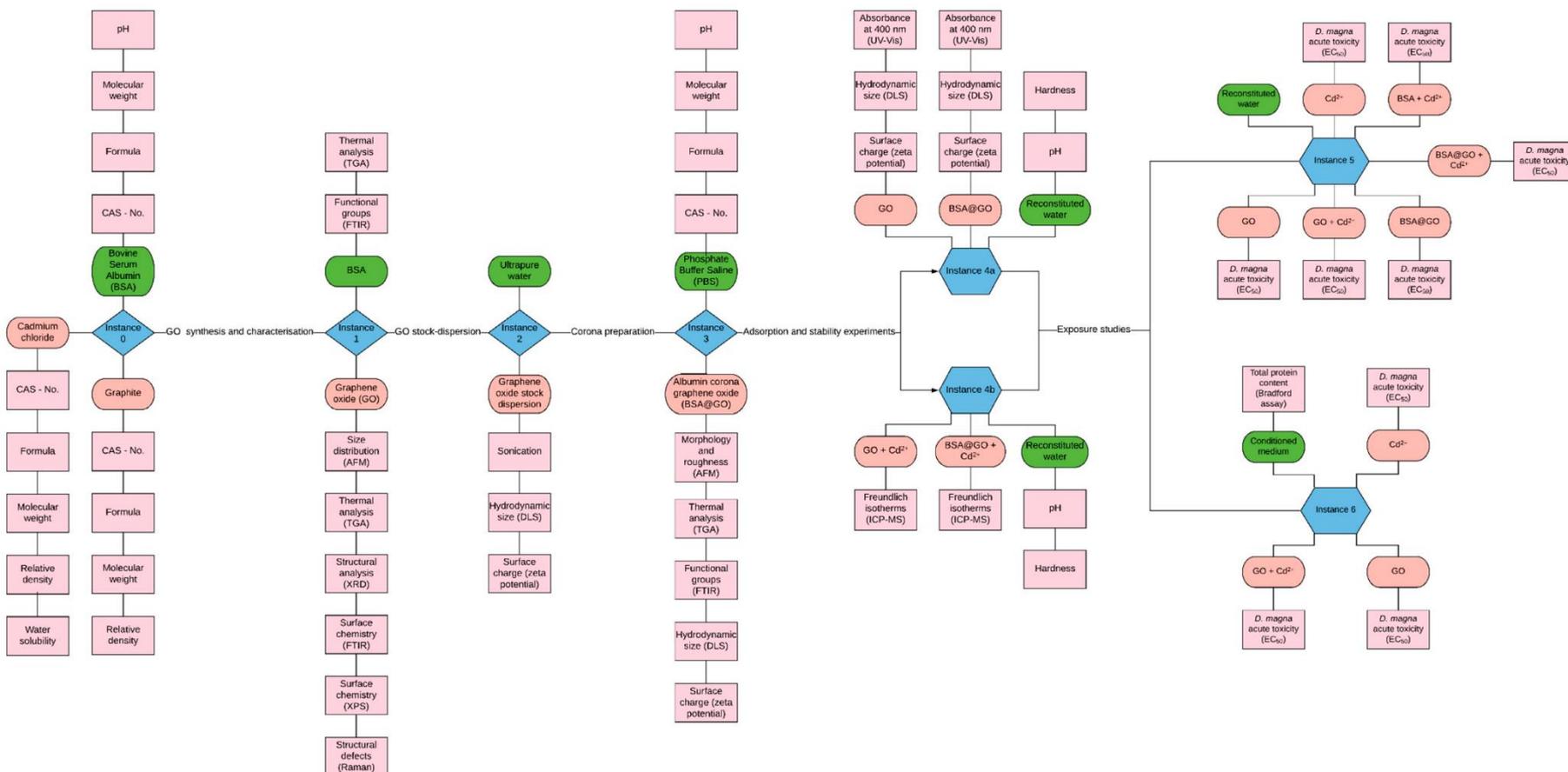
Completed on 08/30/2018

Completed



Electronic laboratory notebooks

Let's go back



Electronic laboratory notebooks

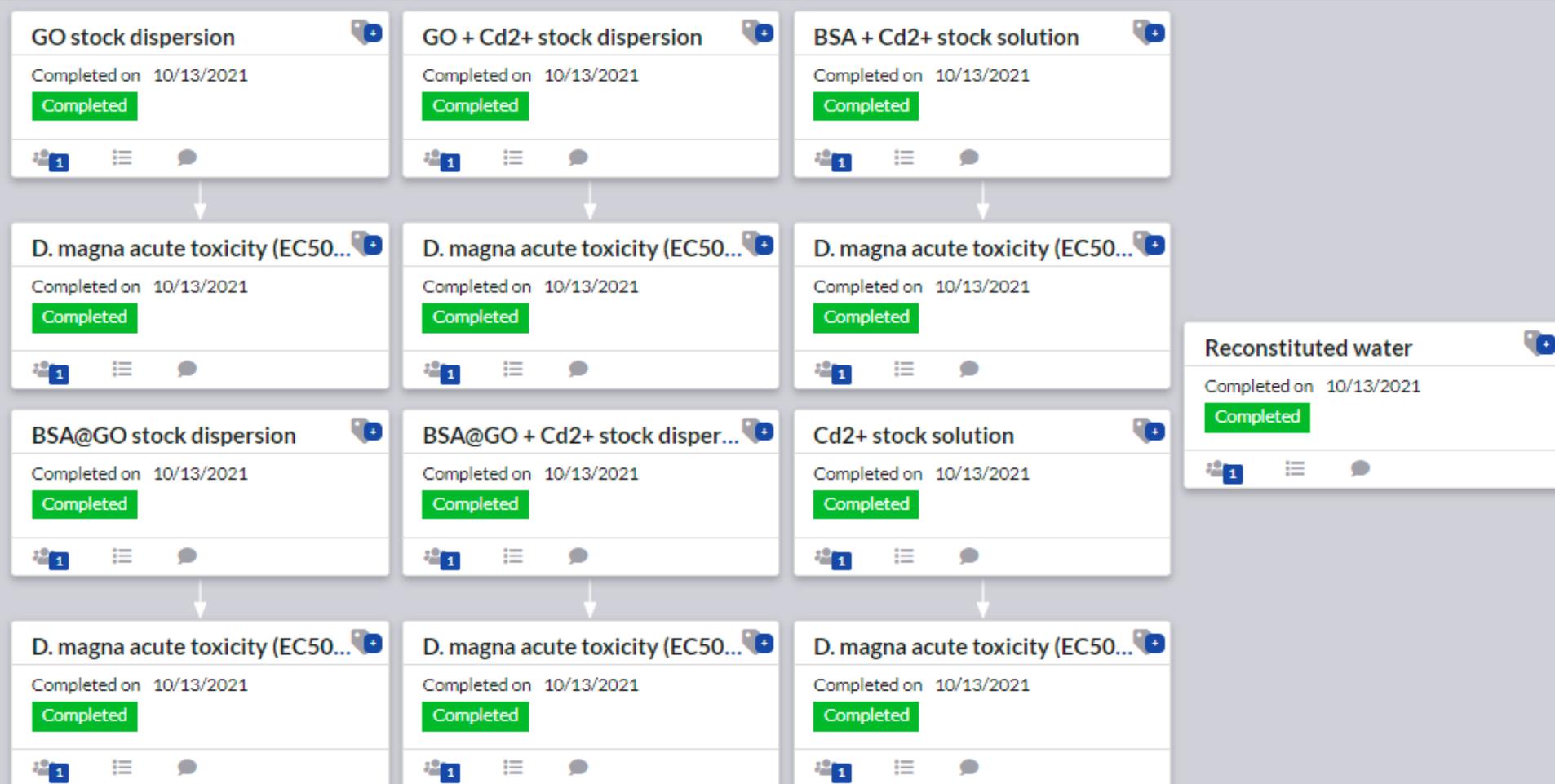
Projects /
GO-Cd-Daphnia

View ▾ 1F

+ New experiment

<p><input type="checkbox"/> Clone 1 - Instance 0 - Starting materials: CdCl₂, Graphite, BSA</p> <p>Start date 10/14/2021</p> <p>Modified date 10/14/2021</p> <p>Completed 0/3 tasks</p> <p>General information on the Cadmium Chloride used during the experimental process. more</p>	<p><input type="checkbox"/> Instance 6 - Toxicity assessment in conditioned medium</p> <p>Start date 05/20/2020</p> <p>Modified date 10/13/2021</p> <p>Completed 7/7 tasks</p> <p>Acute toxicity assessment of Cd²⁺, GO, and mixtures on Daphnia magna in conditioned medium. more</p>	<p><input type="checkbox"/> Instance 5 - Toxicity assessment in reconstituted water</p> <p>Start date 05/20/2020</p> <p>Modified date 10/13/2021</p> <p>Completed 13/13 tasks</p> <p>Acute toxicity assessment of Cd²⁺, GO, BSA@GO, and mixtures on Daphnia magna in reconstituted water. more</p>	<p><input type="checkbox"/> Instance 4B - Cadmium adsorption experiments</p> <p>Start date 05/20/2020</p> <p>Modified date 10/13/2021</p> <p>Completed 5/5 tasks</p> <p>Adsorption of Cd²⁺ onto bare GO and BSA@GO materials in reconstituted water</p>	<p><input type="checkbox"/> Instance 4A - GO and BSA@GO dispersion stability</p> <p>Start date 05/20/2020</p> <p>Modified date 10/13/2021</p> <p>Completed 9/9 tasks</p> <p>Monitoring the dispersion stability of bare GO and BSA@GO in ultrapure water and reconstituted water. more</p>
<p><input type="checkbox"/> Instance 3 - BSA@GO preparation and characterisation</p> <p>Start date 05/20/2020</p> <p>Modified date 10/13/2021</p> <p>Completed 7/7 tasks</p> <p>Preparation and characterisation of the bovine serum albumin corona coated graphene oxide (BSA@GO). more</p>	<p><input type="checkbox"/> Instance 2 - GO stock-dispersion preparation</p> <p>Start date 05/20/2020</p> <p>Modified date 10/13/2021</p> <p>Completed 1/1 tasks</p> <p>Preparation of graphene oxide dispersion in ultrapure water</p>	<p><input type="checkbox"/> Instance 1B - BSA characterisation</p> <p>Start date 05/20/2020</p> <p>Modified date 10/13/2021</p> <p>Completed 2/2 tasks</p> <p>Characterisation of BSA (starting material)</p>	<p><input type="checkbox"/> Instance 1A - GO synthesis and characterisation</p> <p>Start date 05/20/2020</p> <p>Modified date 10/13/2021</p> <p>Completed 8/8 tasks</p> <p>Wet synthesis of graphene oxide and physicochemical characterisation</p>	<p><input type="checkbox"/> Instance 0 - Starting materials: CdCl₂, Graphite, BSA</p> <p>Start date 05/20/2020</p> <p>Modified date 10/13/2021</p> <p>Completed 3/3 tasks</p> <p>General information on the Cadmium Chloride used during the experimental process. more</p>

Electronic laboratory notebooks



Electronic laboratory notebooks

Keep in mind

- ELNs are better than paper notebooks
- ELNs are not a complete data management solution
- ELNs should be part of a data management ecosystem
- ELNs are to be used in conjunction with knowledge bases, semantic annotation etc.
- More work is needed to integrate all the different parts and create a fully functional working environment



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Thank you

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