Managing Sample Characterizations - 2021-06-24

Access to sample characterizations

If you have read-only permissions, see Access the Sample Characterization Summary. If you are a curator with appropriate security permissions, you can create, update, and delete characterizations.

This chapter describes how to review or ascribe characterizations to samples save in caNanoLab. Topics in this chapter include:

- Sample Characterization Overview
 - Accessing the Sample Characterization Summary
 - Submitting Characterizations
 - Exporting Sample Information to JSON or XML
- Adding a Physico-Chemical Characterization
 - Defining Physico-Chemical Characterization Properties
- Adding an In Vitro Characterization
 - Defining In Vitro Characterization Properties
- Adding an In Vivo Characterization
- Adding an Ex Vivo Characterization
- Adding an Other Ex Vivo Characterization
- Adding Information to a Characterization
 - Defining the Characterization
 - Defining Characterization Design and Methods
 - Adding Data Findings to a Characterization
 - Adding Supporting Documents to a Characterization
 - Copying to Samples in the Same Primary Organization
- Additional Characterization Tasks
 - Printing Characterization(s)
 - Exporting Characterization(s) to a Spreadsheet
 - Editing a Characterization
 - Deleting a Characterization

Sample Characterization Overview

Sample characterization describe distinctive characteristics or essential features of the sample determined through analytical methods and records information associated with sample properties. Samples can be characterized in caNanoLab by physical or chemical characteristics or by data derived under *in vitro* and *in vivo* conditions.

With the appropriate security permissions...

With the appropriate security permissions, you can

- Add a Physico-Chemical, In Vitro, In Vivo, Ex Vivo, or Other Ex Vv to a sample.
- Print, export, edit, copy, or delete a characterization and add a file to a characterization.

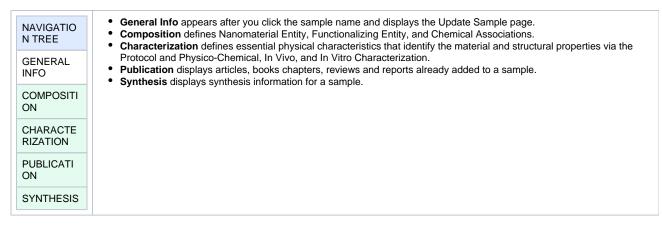
If the buttons do not display, you have read-only access to the item.

Accessing the Sample Characterization Summary

With read-only access, you can review a summary of characterization information and annotations added to the sample.

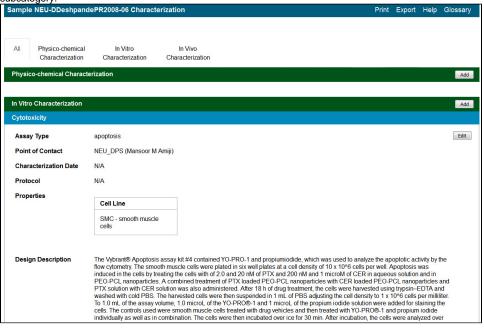
To access characterization functions in the Navigation Tree

- 1. Click Samples and Search Existing Samples.
- 2. Fill in criteria, and click Search.
- 3. Click Edit in the search results.
- 4. The Navigation Tree appears on the left sidebar and comprises functions which you can use to add annotations to the sample.



5. Click Characterization.

The All tab displays characterizations already added to the sample by category. Additional tabs show annotations added to the sample for each subcategory.



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Submitting Characterizations

Once you access Characterizations in the Navigation Tree, you can add different types of information to the sample.

- Adding a Physico-chemical Characterization
- Adding an In Vitro Characterization
- Adding an In Vivo Characterization
- Adding an Ex Vivo Characterization
- Adding an Other Ex Vivo

If you have read-only access, you can View a Characterizations Summary.



To enter an alternative to an option, select other if available and enter a value. The value is added to the list of options.

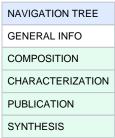
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Exporting Sample Information to JSON or XML

You can export a sample's general information, composition, characterization, publication, and synthesis information to JSON or XML.

To export sample information from the Navigation Tree

1. From the Navigation Tree, select General Info.



2. Click Export (JSON) or Export (XML).



3. The system prompts you to download the information and specify a download location.

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Adding a Physico-Chemical Characterization

To add a physico-chemical characterization

- 1. Access a sample and characterization.
- 2. Click the All tab or the Physico-Chemical Characterizations tab and click Add next to Physico-chemical Characterization.
- $\textbf{3.} \ \ \textbf{Both tabs provide customizations based on your \textbf{Characterization Type}* selection.}$
- 4. Follow these steps to fill in the characterization. Links are provided for additional details.

Section	What to Do
Physico-Chemical Characterization	Fill in the general information about the characterization.
	Note: When you are defining the characterization, to select an existing, non-standard Assay Type, select the Characterization Name, other_pc
Properties	If you select one of the following characterization types, you need to fill in additional properties. Physical State Shape Solubility Surface
Design and Methods	Complete the fields describing techniques and instruments used to derive the data.
Finding	Add data findings and supporting documentation relating to the sample. Import as many .csv files as you wish or add derived data manually.
	Click Add to expand the section, and add data findings and add supporting documents to the characterization.
Analysis and Conclusion	Enter any relevant analyses and conclusions reached by the data.
Copy to Other Samples with the Same Primary Organization	Select samples in the list to which you want this physico-chemical data transferrred. This option copies files and data to one or more selected samples "owned" by the same point of contact.

When you are finished, click **Submit** to save the data to the sample.

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Defining Physico-Chemical Characterization Properties

If you selected one of the Characterization Names listed in the following table, the **Properties** section opens, and you must fill in additional information.

Characterization Name	Properties to Complete
Physical State	Select the Type of physical state. Unknown macro: 'hide'

Shape	1. Select the Type of shape. 2. Enter the shape Aspect Ratio . 3. Enter the Minimum and Maximum Dimensions of the sample, and the units of measurement.	
Solubility	 Select from the options or enter the name of the Solvent. Enter appropriate values for the Critical Concentration, then select the appropriate units for those values. Specify Yes or No to indicate whether the solvent Is Soluble? 	
Surface	Specify Yes or No to indicate whether the surface Is Hydrophobic?.	

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Adding an In Vitro Characterization

In vitro characterization allows you to add characterizations for the nanomaterial component of the sample derived from analytical techniques performed under *in vitro* conditions.

To add an in vitro characterization

- 1. Access a sample and characterization.
- 2. Click the All tab or the In Vitro Characterizations tab and click Add next to In Vitro Characterization.
- 3. Both tabs provide customizations based on your Characterization Type* selection.
- 4. Follow these steps to fill in the characterization. Links are provided for additional details.

Section	What to Do	
In Vitro Characterization	Fill in the general information about the characterization.	
	Note: When you are defining the characterization, to select an existing, non-standard Assay Type, select the Characterization Name, other_vt.	
Properties	If you select one of the following characterization names, you need to fill in additional properties.	
	 Cytotoxicity Enzyme Induction Transfection 	
Design and Methods	Complete the fields describing techniques and instruments used to derive the data.	
Finding	Add data findings and supporting documentation relating to the sample. Import as many .csv files as you wish or add derived data manually.	
	Click Add to expand the section, and add data findings and add supporting documents to the characterization.	
Analysis and Conclusion	Enter any relevant analyses and conclusions reached by the data.	
Copy to Other Samples with the Same Primary Organization	Select samples in the list to which you want this physico-chemical data transferred. This option copies files and data to one or more selected samples "owned" by the same point of contact.	

When you are finished, click **Submit** to save the data to the sample.

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Defining In Vitro Characterization Properties

If you selected one of the Characterization Names listed in the following table, the Properties section opens, and you must fill in additional information.

Characterization Name	Properties to Complete
Cytotoxicity	Enter the appropriate Cell Line.
Enzyme Induction	Enter the Enzyme Name of your choice.
Targeting	Enter the appropriate Cell Line.
Transfection	Enter the appropriate Cell Line.

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Adding an In Vivo Characterization

In vivo characterization allows you to add characterizations for the nanomaterial component of the sample that were derived from analytical techniques performed under *in vivo* conditions.

To add an in vivo characterization

- 1. Access a sample and characterization.
- 2. Click the All tab or the In Vivo Characterizations tab and click Add next to In Vivo Characterization.
- 3. Both tabs provide customizations based on your Characterization Type* selection.

Follow these steps to fill in the characterization. Links are provided for additional details.

Section	What to Do	
In Vivo Characterization	Fill in the general information about the characterization.	
	Note: When you are defining the characterization, to select an existing, non-standard Assay Type, select the Characterization Name, other_vv .	
Design and Methods	Complete the fields describing techniques and instruments used to derive the data.	
Finding	Add data findings and supporting documentation relating to the sample. Import as many .csv files as you wish or add derived data manually.	
	Click Add to expand the section, and add data findings and add supporting documents to the characterization.	
Analysis and Conclusion	Enter any relevant analyses and conclusions reached by the data.	
Copy to Other Samples with the Same Primary Organization	Select samples in the list to which you want this physico-chemical data transferred. This option copies files and data to one or more selected samples "owned" by the same point of contact.	

^{4.} When you are finished, click **Submit** to save the data to the sample.

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Adding an Ex Vivo Characterization

To add an ex vivo characterization

- 1. Access a sample and characterization.
- 2. Click the All tab or the Ex Vivo Characterizations tab and click Add next to Ex Vivo Characterization.
- 3. Both tabs provide customizations based on your Characterization Type* selection.

Follow these steps to fill in the characterization. Links are provided for additional details.

Section	What to Do
Ex Vivo Characterization	Fill in the general information about the characterization.
	Note: When you are defining the characterization, to select an existing, non-standard Assay Type, select the Characterization Name, other_ex_vv
Design and Methods	Complete the fields describing techniques and instruments used to derive the data.
Finding	Add data findings and supporting documentation relating to the sample. Import as many .csv files as you wish or add derived data manually.
	Click Add to expand the section, and add data findings and add supporting documents to the characterization.
Analysis and Conclusion	Enter any relevant analyses and conclusions reached by the data.
Copy to Other Samples with the Same Primary Organization	Select samples in the list to which you want this physico-chemical data transferred. This option copies files and data to one or more selected samples "owned" by the same point of contact.

^{4.} When you are finished, click **Submit** to save the data to the sample.

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Adding an Other Ex Vivo Characterization

To add an other ex vivo characterization

- 1. Access a sample and characterization.
- 2. Click the All tab or the Other Ex Vivo Characterizations tab and click Add next to Ex Vivo Characterization.
- 3. Both tabs provide customizations based on your Characterization Type* selection.

Follow these steps to fill in the characterization. Links are provided for additional details.

Section	What to Do
Other Ex Vivo Characterization	Fill in the general information about the characterization.
Design and Methods	Complete the fields describing techniques and instruments used to derive the data.
Finding	Add data findings and supporting documentation relating to the sample. Import as many .csv files as you wish or add derived data manually.
	Click Add to expand the section, and add data findings and add supporting documents to the characterization.
Analysis and Conclusion	Enter any relevant analyses and conclusions reached by the data.
Copy to Other Samples with the Same Primary Organization	Select samples in the list to which you want this physico-chemical data transferred. This option copies files and data to one or more selected samples "owned" by the same point of contact.

4. When you are finished, click Submit to save the data to the sample.

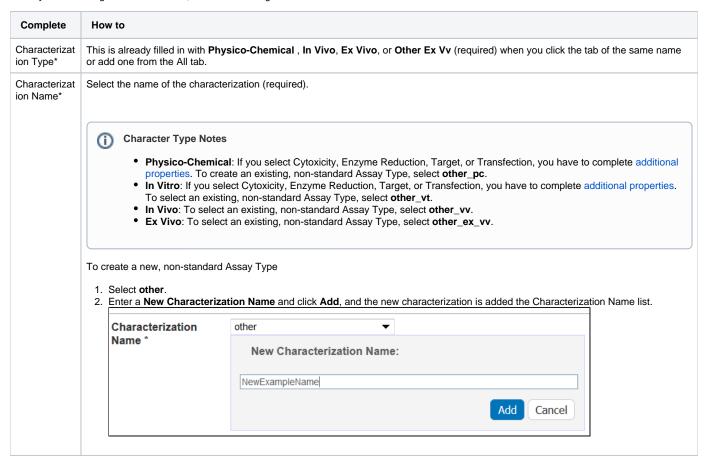
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Adding Information to a Characterization

The following procedures apply to any Characterization Type when you are adding or editing a characterization.

Defining the Characterization

When you are adding a characterization, fill in the following characterization information.



Assay Type	Select an assay type from the list that populates automatically based on the Characterization Name.	
	To add an Assay Type	
	 Select other. Enter a New Assay Type and click Add, and t he new Assay Type is added to the list. 	
Protocol Name – Version	If available, select a protocol from which the data is derived. If displayed, click the hyperlink to the protocol text file to open or save the file.	
Characterizat ion Source	Select or enter the source from which the characterization data is derived, such as a vendor or a laboratory (NCL).	
Characterizat ion Date	Select or enter the date the characterization was made (dd/mm/yyyy).	

Defining Characterization Design and Methods

When you are adding a characterization, fill in the following design, methods, and techniques used.

Design and Methods Field	Description	
Design and Methods Description	Enter a description for the characterization design and methods.	
	Adding extra lines If you include an extra line between text in the Characterizations free text, Design and Methods Description, the line separation is preserved when you save or update the characterization.	
Technique and Instrument	Click Add to expand the page where you can select and enter information regarding the technique and instrument used to derive the sample.	
Technique*	Select the technique (required).	
Abbreviation	When you select a technique, Abbreviation populates automatically if an abbreviation is known. If not, enter an abbreviation.	
Description	Enter a description of the technique and instrument.	
Instrument	Click Add to expand the Instruments panel. Enter or select identifying information about the instrument used to obtain data. • Select the instrument Manufacturer . • Enter the instrument Model Name . • Enter the model Type .	

When you are finished, click Save or Cancel to close the section without saving.

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Adding Data Findings to a Characterization

To add findings to a characterization, you can add data directly to Data and Conditions by creating columns and adding data manually or you can import as many .csv files as needed. Information can include laboratory conditions, pH, or temperature. You can add as many files as you wish.

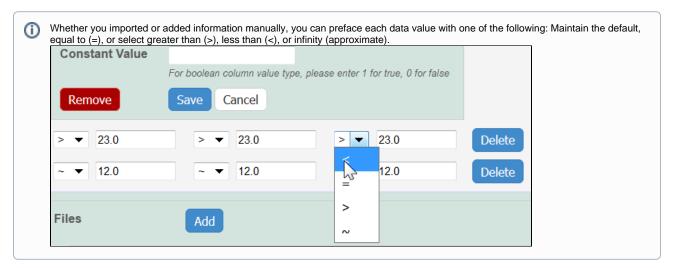
- 1. Add data values to Data and Conditions.
 - a. To import a file of data values
 - i. Save the spreadsheet of data values to a csv (comma-separated value) file.
 - ii. Click Import csv and select and follow the prompts to add the data file to the Findings Info.



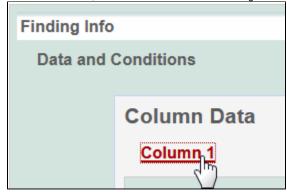
- iii. The columns and data are added to Data and Conditions.
- **b.** To add the data values manually
 - i. Specify the number of columns and rows for the matrix, and click Update.



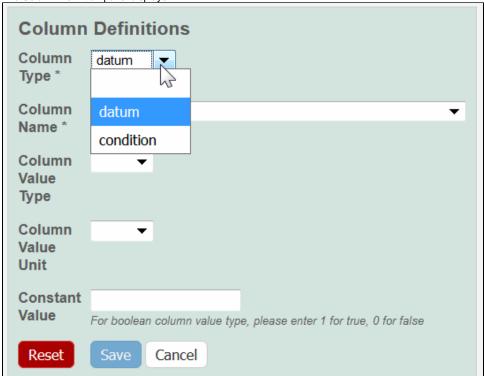
ii. Add the data values to the rows.



2. To define a column, click an underlined column heading.



The Column Definition panel displays.



- 3. Select a Column Type, Datum or Condition.
- 4. Select a Column Name or select other and add a new one.

(ii)

Column Notes

You can add up to three cell viability Column Names, including **cell viability**, **cell viability B**, and **cell viability C**. You can further identify the column with the Column Value Type.

a. For Column Type, Datum, the following characterization(s) display customized Column Name options.

Characterization Type	Column Type and Column Name Option(s)	
Physico-Chemical	 Molecular – Molecular Weight Purity – % purity for sample Relaxivity – R1, R2, T1, T2 Size – PD1, Peak N, RMS size, Z Average Surface – charge, zeta potential 	
In Vitro	Enzyme Induction – % of Control	
In Vivo	Click Other to name the column yourself.	

b. For Column Type, **Condition**, all characterizations provide the **Column Name** options in the left column of the following table. The Column Name autopopulates the **Condition Property** options in the right column.

Column Type, Condition Autopopulates Column Name	Column Name Autopopulates Condition Property
Centrifugation	N/A
Culture Media	media type, serum percentage
Electromagnetic Radiation	bandwidth, frequency, time, wavelength
Freeze Thaw	N/A
Long Term Storage	lyophilized, time
Lyophilization	time
рН	N/A
Sample concentration	N/A
Short Term Storage	lyophilized, time
Solvent Media	ion concentration, ionic strength, molecular formula, osmolality, serum percentage, with serum
Sonication	number of pulses, pulse duration
Temperature	N/A

5. To further identify a column, select a Column Value Type.



Once the column information is saved, the Column Type is shown in parentheses after the Column Name, such as **cell viability** (mean).

- 6. Select a Column Value Unit, or select other and add one.
- 7. If you want the same value to fill all rows in a column, add a Constant Value.
 - **①**

For Column Value Type, boolean

For Column Value Type, boolean, enter a Constant Value of 1 for true and 0 for false.

8. Click Save, and the column(s) are updated.



If needed, click Set Column Order to change the order of the column headings in the matrix.

9. Click Save in the Finding section.

Adding Supporting Documents to a Characterization

To add results in the form of supporting documents, such as a graphic, spreadsheet or images to a characterization



You can add as many files as you wish.

- 1. In the Finding section of the characterization, next to Files, click Add.
- 2. Upload, browse, and select the file or enter the file's URL where the document is located.
- 3. Complete the following.
 - a. Select the File Type (required), Document, Graph, Image, Movie, or Spreadsheet.
 - b. Enter the File Title (required).
 - c. Specify Keywords to associate with the file
 - d. Enter a Description of additional information of the file.
- 4. Click Submit to add the file(s) to the sample.

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Copying to Samples in the Same Primary Organization

The composition files and/or derived data for a sample can be copied to other samples from the same primary point of contact.

- 1. From the All tab's characterizations summary, click Edit at the right of a characterization section.
- 2. The Characterization opens and at the bottom of the page, in the Copy to other samples... section, select one or more samples with the same primary point of contact.
- 3. Click Also copy finding data and conditions?.
- 4. Click **Submit** to copy the characterization.

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Additional Characterization Tasks

The following table lists tasks that require Curator privileges.



If a button does not display, you have read-only access to the data.

Task	How to
Printing Characterization(s)	To print the characterization(s), from the All tab characterization summary, click Print at the top right of the page.
Exporting Characterization (s) to a Spreadsheet	To export the characterization(s) to a spreadsheet, from the All tab characterization summary, click Export at the top right of the page. To export all sample information to JSON or XML, see Exporting Sample Information to JSON or XML
Editing a Characterization	 From the All tab's characterizations summary, click Edit at the right of the characterization section you want to change. The Characterization opens and you can edit it as needed.

Deleting a Characterization



Deleting a characterization

This deletes a characterization(s) from the selected sample. If the characterization(s) was copied to other samples, the characterization is not removed from those samples.

To delete a characterization for a selected sample

- From the All tab's characterizations summary, click Edit at the right of a characterization section.
 The Characterization opens, and click Delete.
- 3. The deleted characterization is placed in the sample archive for historical purposes.

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