Managing Sample Composition Annotations - 2021-06-24

> **Access to sample compositions**
>
> If you have read-only permissions, see Accessing the Sample Composition Summary. If you are a curator with appropriate security permissions, you can perform all the tasks described in this chapter.

This chapter describes how to manage the samples' information accessible from the Navigation Tree. Topics in this chapter include

Sample Composition Overview

Sample composition records information associated with the way a sample is made, especially in terms of its different parts, its constituents. Composition for a sample in caNanoLab consists of information categorized by nanomaterial entity, functionalizing entity, and chemical association(s). You can also add files relevant to the sample composition or derivation of its data.

- **Nanomaterial Entity** composition describes the component of a sample that is a nanoparticle.
- **Functionalizing Entity** composition describes the substance, physical or biological factor, etc. of the sample that produces a specific effect.
- **Chemical Association** composition annotations describes the chemical association(s) of the nanoparticle/functionalizing entities of the sample.
- **Composition File** enables you to add files relevant to the sample independently of the entity or chemical associations.

Accessing the Sample Composition Summary

If you have read-only access, you can review the sample composition summary.

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.

NAVIGATION TREE	
GENERAL INFO	**General Info** appears after you click the sample name and displays the Update Sample page. **Composition** defines Nanomaterial Entity, Functionalizing Entity, and Chemical Associations. **Characterization** defines essential physical characteristics that identify the material and structural properties via the Protocol and Physico-Chemical, In Vivo, and In Vitro Characterization. **Publication** displays articles, books chapters, reviews and reports already added to a sample. **Synthesis** displays synthesis information for a sample.
COMPOSITION	
CHARACTERIZATION	
PUBLICATION	
SYNTHESIS	

5. Click **Composition.**
   The **All** tab displays compositions already added to the sample by category. Additional tabs show items added to the sample for each subcategory.

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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 Nanomaterial Entity Composition Annotations

To add a nanomaterial entity

1. Access a sample and composition.
2. Click the **Nanomaterial Entity** tab or the **All** tab and click **Add** next to Nanomaterial Entity.
3. Both tabs provide customizations based on your **Nanomaterial Entity Type*** selection.

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

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

Section	What to Do
Nanomaterial Entity Type*	Select the entity type (required) and add a **Description** for the entity. **Note:** Entity types are described in the caNanoLab Glossary.
Properties	If you select one of the following entity types, you need to fill in additional Properties. • Bipolymer • Carbon Nanotube • Dendrimer • Emulsion • Fullerene • Lipsome • Polymer
Composing Element	Add information regarding the elements that compose the nanomaterial entity of the sample.
File	Click **Add** to expand the page to add one or more files whose data is relevant to the nanomaterial entity or the derivation of its 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 Nanomaterial Entity Properties

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

Nanomaterial Entity Type	Properties to Complete
Biopolymer	1. If you are defining a Nanomaterial Entity, enter the **Name** of the biopolymer. 2. Select the **Biopolymer type** of antibody functionalizing entity for this sample. 📄 Unknown macro: 'hide' 3. Using the appropriate format, enter the complete **Sequence** of the biopolymer.
Carbon Nanotube	1. Enter the **Average Length** of the nanotube. 2. Enter the **Length Unit** of measurement for the average length measurement of the nanotube. 3. The spatial position or orientation of functional groups located within a molecule. • Enter information about the **Chirality** in the nanotube and its effect on the orientation of functional groups located on the particle. 4. Enter the measurement of the nanotube **Diameter**, as measured from one side of the tube wall through the center of the nanotube to the opposite point on the circumference. 5. Enter the **Diameter Unit** of measurement for the nanotube diameter. 6. Select the appropriate description of the nanotube **Wall Type**. • **DWNT** (Double-Wall Nanotube) Nanotube wall consists of two layers of graphitic carbon. • **MWNT** (Multiple-Wall Nanotube) Nanotube consists of single-walled nanotubes layered inside each other • **SWNT** (Single-wall Nanotube) Wall consists of a single layer of graphitic carbon

Dendrimer	Branches are molecules that branch off of the core (like tree branches). • Enter a description that represents the number of **Branches** in the dendrimer. Generations are shells layered on the core of a dendrimer. Dendrimers consist of layers of chemical shells built on a core module. Each shell consists of two chemicals in the same order (A-B) and each shell is called a generation. The generations are labeled in decimal to illustrate the shell layering/consistency. For example, Generation 2.5 (G2.5) = 1 shell of A-B (1), surrounded by a second shell of A-B (2), topped off with only one chemical A within the shell (.5). As such, the layering structure would be (A-B, A-B, A) = 2.5. • List the **Generations** reflected in this dendrimer.
Emulsion	1. Specify whether the emulsion **Is Polymerized** (required). Polymerization consists of enzymatic reactions that link a series of monomers, forming a polymerized compound (polymer), usually of high molecular weight, by combination of simpler molecules (monomers). 2. Enter the name of the polymer (**Polymer Name**) suspended in the emulsion (required).
Fullerene	1. Enter the **Average Diameter** measurement, as measured from one side of the nanoparticle through its center to the opposite point on the circumference. 2. Enter the **Average Diameter Unit** of measurement for the fullerene diameter. 3. Enter the **Number of Carbon** molecules comprising the fullerene.
Liposome	1. Enter the name of the liposome polymer (**Polymer Name**). 2. Polymerization consists of enzymatic reactions that link a series of monomers, forming a polymerized compound (polymer), usually of high molecular weight, by combination of simpler molecules (monomers). • Specify Yes or No to indicate whether the liposome Is **Polymerized** or not (require).
Polymer	1. In **Initiator** , enter the agent that initiated the polymerization**.** Examples are free radicals or peroxide. 2. Crosslinking is a covalent bond between two polymers or two different regions of the same polymer. • Specify Yes or No to indicate whether the polymer **Is Crosslinked**. 3. In **Crosslink Degree**, enter the percentage level of covalent linkage in the polymer.

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Defining Nanomaterial Composing Elements

Define the following composing elements for the nanomaterial entity.

Complete	How to
Composing Element Type*	Select the type of composing element comprising this nanomaterial (required). Unknown macro: 'hide'
Chemical Name*	Enter the chemical name given to the atomic or molecular structure that composes the center of the nanoparticle (required).
Crosslink Degree	Enter the percentage level of covalent linkage in the polymer.
PubChem Data Source /PubChem ID	Select one of the three PubChem data sources: **Compound**, **Substance**, or **BioAssay**. The database is located here: http://pubchem.ncbi.nlm.nih.gov/. Enter the **PubChem ID** which is the PubChem identifier for a compound, a substance, or a bioassay.
Amount/Amount Unit	Select the appropriate values and unit for this composing element information.
Molecular Formula Type	Select the molecular formula type found in this biopolymer. • Hill • SMARTS • SMILES
Molecular Formula	Enter the chemical formula of the nanoparticle.
Description	Enter a description for the composing element.

Inherent Function	Inherent function is the characteristic behavior of a sample that results from the chemical and physical composition and properties of the entity.
	Click **Add** to expand the page where you can enter this information.
Function Type	Select the function type category which best fits the nanomaterial entity.
	ⓘ If you select **imaging function**, you must specify an Imaging Modality Type.
	📖 Unknown macro: 'hide'
Description	Enter any additional function information for the nanomaterial entity that the form does not already include.

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

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Adding Functionalizing Entity Composition Annotations

To add a functionalizing entity

1. [Access a sample and composition].
2. Click the **Functionalizing Entity** tab or the **All** tab and click **Add** next to Functionalizing Entity.
3. Both tabs provide customizations based on your **Functionalizing Entity Type*** selection.

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

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

Section	What to do
Functionalizing Entity	Fill in the general information about the functionalizing entity.
	Note: Entity types are described in the [caNanoLab Glossary].
Properties	If you selected one of the following entity types, you need to fill in additional properties.
	• Antibody
	• Bipolymer
	• Small Molecule
Inherent Function	Add information about the functionalizing elements of the sample.
File	Add one or more files containing data that is relevant to the functionalizing entity or the derivation of its data.
Copy to Other Samples with the Same Primary Organization	Select one or more samples in the list to which you want this composition 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 a Functionalizing Entity

Fill in the following functionalized entity information.

Complete	How to
Entity Type	Select the functionalizing entity type.
	Note: Entity types are described in the [caNanoLab Glossary].
Chemical Name	Enter the chemical name for the functionalizing entity whose type you just selected.

PubChem Data Source /PubChem ID	Select one of the three PubChem data sources: **Compound**, **Substance**, or **BioAssay**. The database is located here: http://pubchem.ncbi.nlm.nih.gov/. Enter the **PubChem ID** which is the PubChem identifier for a compound, a substance, or a bioassay.
Amount/Amount Unit	Select the appropriate values and unit for this composing element information.
Molecular Formula Type	Select the molecular formula type found in this biopolymer. • Hill • SMARTS • SMILES
Molecular Formula	Enter the chemical formula of the functionalizing entity.
Activation Method	Select the method used to activate the functionality of the sample from the list. ⓘ If you do not have to activate the entity, select **does not require activation**. 📋 Unknown macro: 'hide'
Activation Effect	Enter the functional effect of the entity.
Description	Enter any additional composition information that the form does not include.

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

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Defining Functionalizing Entity Properties

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

Functionalizing Entity Type	Properties to Complete

Antibody	1. Select the **Type** of antibody functioning for this sample.
	   • Fab
	   • ScFv
	   • whole
	2. Select the **Isotype** for this antibody.
	   • IgA
	   • IgD
	   • IgE
	   • IgG
	   • IgM
	3. Select the animal **Species** from which the antibody was derived.

Biopolymer	1. Select the **Biopolymer type** of antibody functionalizing entity for this sample. 📋 Unknown macro: 'hide' 2. Using the appropriate format, enter the complete **Sequence** of the biopolymer.
Small Molecule	Add an **Alternate Name** for the Small Molecule.

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Defining Function Information

Fill in the following inherent function information for the functionalizing entity.

Complete	How to

ⓘ

Function Type	Select the function type category which best fits the nanomaterial entity.
	(i) If you select **imaging function**, you must specify an Imaging Modality Type.
	📖 Unknown macro: 'hide'
Description	Enter any additional composition information that the form does not include.

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

(i) In the Navigation Tree, a hyperlink for the new Composition characterization is added under the Functionalizing Entity.

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Adding Chemical Association Composition Annotations

You can enter basic annotation information describing the chemical association(s) of the sample and/or functionalizing entities of the sample.

(i) **Chemical association requirement**

To enter chemical association information, you must enter at least two composing elements and/or at least one functionalizing entity to the sample entity.

To add a chemical association

1. Access a sample and composition.
2. Click the **Chemical Association** tab or the **All** tab and click **Add** next to Chemical Association.
3. Both tabs provide customizations based on your **Association Type*** selection.
4. Follow these steps to fill in the association. Links are provided for additional details.

Complete	How to
Association Type*	📖 Unknown macro: 'hide' Select a chemical association type (required).
Description	Enter any additional information that describes the chemical association of the two elements.
Element	In the Elements Information section, both **Element** boxes list the nanomaterial or functionalizing entities you defined while annotating the sample. a. Each time you select an option, a list displays entities relating to your previous selection. b. Select an option from each list. The arrow between the Element text boxes symbolizes the association between the two.
File	Click **Add** to expand the page where you can add one or more files whose data is relevant to the functionalizing entity or the derivation of its data.

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

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Adding Information to the Composition

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

Adding Composition Files

You can add results in the form of supporting documents, such as a graphic, spreadsheet or images, to a sample or files relevant to the sample independent of the entity or chemical associations that you defined.

To add files to a sample

1. Access a sample and composition.
2. To add a file, click the **Composition File** tab or the **All** tab and scroll to the File section.
3. Click **Add** next to File.

4. Upload, browse, and select the file or enter the file's URL where the document is located.
5. 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.
6. When you are finished, click **Submit** to add the file(s) to the sample.

> ✅ **Editing and Deleting a File**
>
> Once you add a composition file, you can remove the file or edit the composition file information.
>
> To delete a file, click **Delete**.
>
> To update the file information, click **Edit** and on the Edit Composition File page, make the changes and click **Update**. The list of files is updated.

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 composition section.
2. The Composition 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. When you are finished, click **Submit** to copy the composition.

Additional Composition 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 a Composition(s)	To print the composition(s), from the **All** tab composition summary, click **Print** at the top right of the page.
Exporting Composition(s) to a Spreadsheet	To export the composition(s) to a spreadsheet, from the **All** tab composition 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 Composition	1. From the **All** tab's composition summary, click **Edit** at the right of the composition section you want to change. 2. The Composition opens and you can edit it as needed.
Deleting a Composition	> ⓘ **Deleting a composition** > This deletes a composition(s) from the selected sample. If the composition(s) was copied to other samples, the composition is not removed from those samples. To delete a composition for a selected sample 1. From the **All** tab's composition summary, click **Edit** at the right of a composition section. 2. The composition opens, and click **Delete**. 3. The deleted composition is placed in the sample archive for historical purposes.