

The NanoFASE NIKC Curation Manual



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Acknowledgements

This manual has been produced on behalf of NanoFASE in collaboration between:

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The material was developed at the CANICULE (Congress to Advance Nano Informatics Collaborations by Uniting and Leveraging Efforts) workshop at CEREGE, Aix-en-Provence 27-28 June, 2019 between members of:

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This material is based upon work supported by the National Science Foundation (NSF) and the Environmental Protection Agency (EPA) under NSF Cooperative Agreement DBI-1266252, Center for the Environmental Implications of NanoTechnology (CEINT). It was previously funded under NSF Cooperative Agreement EF-0830093. The work was also supported in part via cooperative agreement W912HZ-17-2-0002 between the US Army Corps of Engineer Research and Development Center (USACE ERDC) and the US Consumer Product Safety Commission. Any opinions, findings, conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the NSF, the EPA, the USACE ERDC or the US CPSC. This work has not been subjected to EPA review and no official endorsement should be inferred.

The EU projects [NanoFASE*](#) and [NanoCommons*](#)

Marianne Matzke, Lee Walker, Claus Svendsen from UKRI-Centre for Ecology & Hydrology (UK)

Anastasios (Tassos) Papadiamantis and Iseult Lynch – *University of Birmingham (UK)*

Dieter Maier - *Biomax (DE)*

Thomas Exner – *Edelweiss Connect (CH)*

Geert Cornelis – *Swedish University of Agricultural Sciences (SE)*

**These projects have received funding from European Union Horizon 2020 Programme (H2020) under grant agreement n° 646002 (NanoFASE, 2015-19) and n° 731032 (NanoCommons, 2018-21).*

The [Labex SERENADE](#) Project

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*This work is a contribution to the Labex Serenade (ANR-11-LABX-0064) funded by the French Government's "Investissements d'Avenir" ANR program, through the A*MIDEX project (ANR-11-IDEX-0001-02).*

Introduction to the NIKC Curation Manual

The Nanomaterial Fate and Speciation in the Environment (NanoFASE) project has been funded by the European Commission from 2016-2019 to develop integrated exposure assessment capabilities that successfully predict environmental distribution, concentration, and form (speciation) of nanomaterials. To enable this complex mission, data and model estimates must be amalgamated across a multitude of disciplines, from numerous individual research groups and stakeholders, in a harmonized format that can allow comparison and combined analysis. The Nanomaterial Environment, Health and Safety (NanoEHS) field recognizes, and seeks to address, the fact that exposure modeling and prediction methods developed for use in managing chemical risks cannot be directly ported into the exercise of forecasting nanomaterial behavior. The dynamic physics and chemistry of the particles and the systems they move through mean that initial nanomaterial characterisations may be less useful to predicting exposure than key interactions and transformations the particles undergo. Progress has been made within the emerging field of nanoinformatics to develop shared taxonomies and ontologies, and to harmonize key methods and reporting formats, but finalized standards are far from formal establishment.

The data generated from the NanoFASE project will be curated and housed within the NanoInformatics Knowledge Commons (NIKC), a shared repository available for contributing partners on a global basis. This manual explains how data owners format and enter their data into the NIKC, in conjunction with help from dedicated curator.

The Center for the Environmental Implications of Nano Technology (CEINT), funded by the United States National Science Foundation from 2008-2019, first developed the NIKC as a cyberinfrastructure and associated curation tools providing the capability to follow the spatial-temporal arc of a nanomaterial and its transformations across the experimental timeline, including key information (e.g. surrounding medium characteristics) within the kernel of characterisation. The NIKC has been built incorporating the extensive efforts of the EU-funded eNanoMapper project, which has developed an ontology, and gathered a vast number of terms linked to other extant ontologies. The NIKC team and eNanoMapper team continue to work together, so that as the NanoEHS and nanoinformatics fields move ahead, continual global efforts support convergence, harmonization, and ultimately a critical mass of interoperable data that support multiple missions.

The CEINT NIKC team is partnering with the NanoFASE team, NanoCommons team, and others to fully and transparently share all developed cyberinfrastructure and curated datasets so that multiple data owners whose experiments include meta-data that allow for the interrogation of nanomaterial behavior in complex systems.

Curation is the practice of storing data involving informed-decision making to determine *what information* should be curated, when data curation is *complete*, and how to identify *high-quality* data. Data can be curated by a dedicated curator from literature, but this is not the most efficient approach, and potentially can introduce inaccuracies. The ideal workflow is that experimenters and data owners curate their results into the NIKC database structure using harmonized terminology. (As a bonus, some researchers report that the process of curation has helped them reflect upon completeness of their data and experimental design, and clarify knowledge gaps.)

The purpose of this manual is to provide a structural overview of the NIKC, and explain to data owners the process of curating their own data in partnership with a dedicated curation expert. After completing this manual, readers should understand: 1) the type of data and metadata being curated, 2) the established relationship between media and materials central to the NIKC design, 3) how and when to work with their curator guide to upload their NanoFASE datasets.

An Introduction to NIKC Excel Template

Why use Excel Spreadsheets?

Excel spreadsheets are a common format used by most professionals of all subfields of science and therefore was a reasonable and logical data entry format. To promote wide-spread use of the NIKC database we chose Excel as an easy-to-use software that does not require pre-requisite computing skills. Reference information, experimental results, procedural details, parameter terms are stored in one Excel file in eight spreadsheet tabs. These eight tabs are separated into three broad categories: reference information, measurement, and method. After the Excel template tabs are completed, the database administrator uploads data from the Excel spreadsheets onto the NIKC database.

Excel Spreadsheets Tabs Organization

What information is curated and why is this information important?

Figure 1. Highlighted Spreadsheet Tabs from CEINT NIKC Excel Template with sample data



Reference

Information Spreadsheet Tabs

The reference tabs are essential for linking individual data points to the paper of origin, creating a literature library of work for authors, and providing access to the paper's abstract. Referencing information is separated into three tabs: 1) Publication, 2) Institution, 3) and People.

The People tab catalogs the researchers' names and contact information, while assigning unique IDs to each researcher. The researchers' ID number is kept constant even if the researcher curate multiple datasets and changes institution associations. Affiliated with each researcher's ID is the researchers' corresponding institution. Further information for each institution can be found in the

datasetId	Instance	Registry number	Material	Medium	measurementType	parameter	InherId	parameterDescription	parameterDataType	parameterText	para
01.001/1000	Stock dispersion		Environ CeO2 NP		property	CeO2 concentration		Reported by Experimenter	Numeric		mean
01.001/1000	Stock dispersion		Environ CeO2 NP		property	mean primary particle size		Reported by Experimenter	Numeric		mean
01.001/1000	ID			Sewage sludge	property	Ce concentration		Reported by Experimenter	Numeric		mean
01.001/1000	ID			Sewage sludge	property	Total solids		Reported by Experimenter	Numeric		mean
01.001/1000	II			Sewage sludge	Property	Total solids		Reported by Experimenter	Numeric		
01.001/1000	II		Environ CeO2 NP		Property	Amount		Reported by Experimenter	Numeric		
01.001/1000	IQ			Dry sewage sludge	property	Mass		Reported by Experimenter	Numeric		
01.001/1000	IQ			Dry sewage sludge	property	Ce concentration		Reported by Experimenter	Numeric		mean
01.001/1000	IQ			Dry sewage sludge	property	Ash content		Reported by Experimenter	Numeric		
01.001/1000	IQ			Dry sewage sludge	Property	Total carbon		Reported by Experimenter	Numeric		
01.001/1000	IQ		Environ CeO2 NP		property	KAS		Reported by Experimenter	Numeric		
01.001/1000	IR			Fly Ash	property	Mass		Reported by Experimenter	Numeric		
01.001/1000	IR			Fly Ash	property	Ce concentration		Reported by Experimenter	Numeric		mean
01.001/1000	IR			Fly Ash	Property	Total carbon		Reported by Experimenter	Numeric		

institution tab, where the department, institution, city, state, zip code, and country is recorded. The Publication tab list the DOI and abstract of every dataset that has been curated, which can be accessed by users without needing to refer to the publication. The Publication tab also includes curation notes that informs the reader supplementary information about the curated dataset that the researchers' would like to convey.

Measurement Spreadsheet Tabs

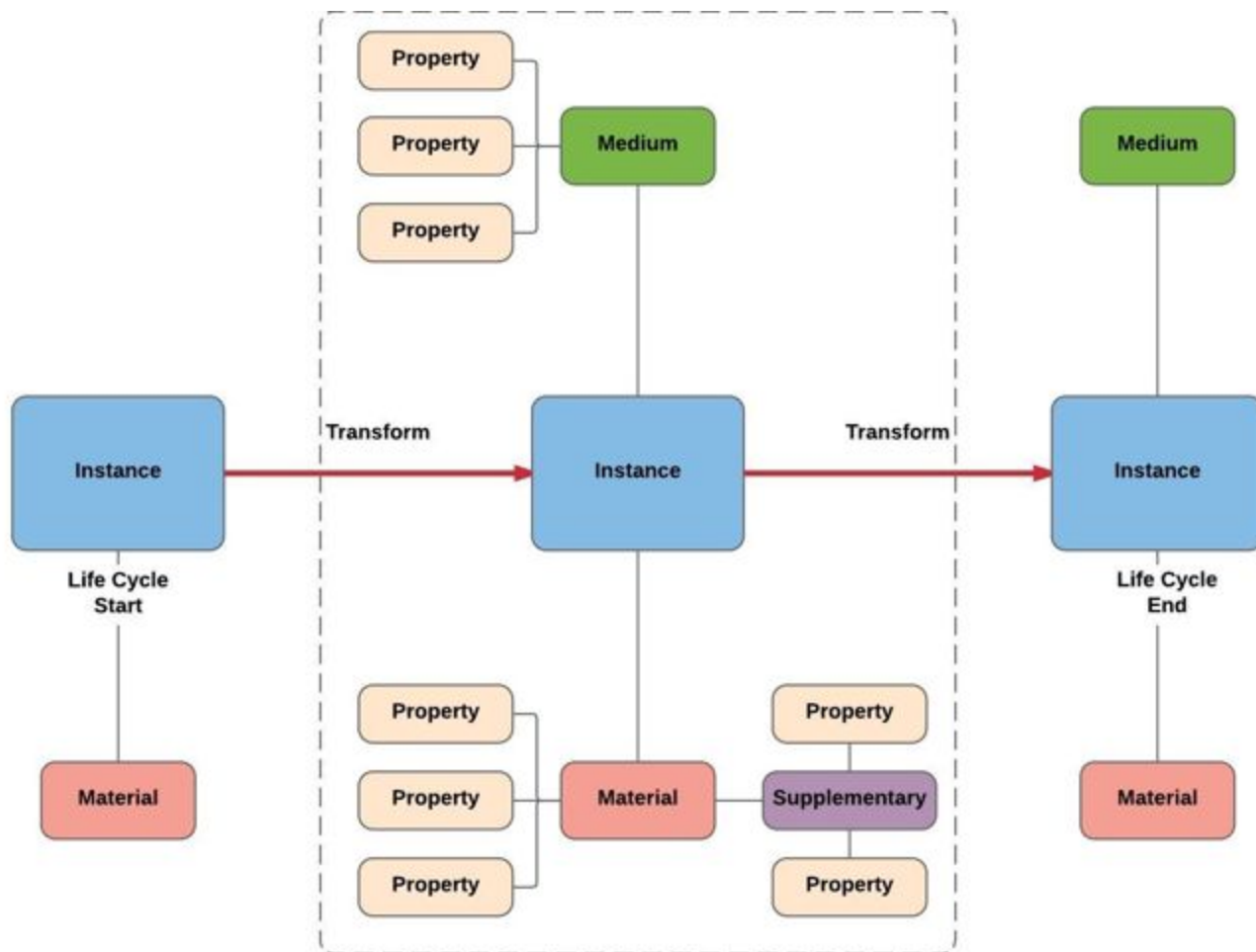
Measurement Tabs consist of the measurement tab and instance tab. The measurement tab is where data is deconstructed and reorganized into the NIKC's database structure. Data and metadata are entered into the measurement and instance tabs, connecting the metadata to the data point that it describes. Metadata collected by the NIKC database includes characterizations about the medium and the nanomaterial. Instance changes due to elapsed time are captured in the time relative, time unit, and time absolute columns located in the instance tab. Endpoints stored by NIKC are dependent on the medium being studied. Mammalian test subject endpoints may include accumulation, biodistribution, or death; however, in mesocosm studies endpoints may include changes in growth, or dissolved oxygen levels. Every datapoint is linked to a protocol and instrument ID when applicable, which allows the user to determine if the method used to achieve the results is relevant for their experiments.

Methods Spreadsheet Tabs

The methods section of the NIKC spreadsheets is separated into a Protocol tab and an Instrument tab. The protocol tab records details of the experimental procedures, including experimental time length, a description of the protocol, and a column for protocol and method references. The protocol tab was designed to allow researchers to record the individual steps within a protocol. The Instrument tab records the instruments used in the experiments listing the model and country of origin. Every new protocol, protocol step, and instrument entry is given an ID, which helps to prevent repetition between curated publications. Similar to the people ID, the ID for an instrument remains constant from publication to publication. For example, if the same instrument make and model is cited in multiple publications from various authors, create one entry with one ID, and link the same ID for each paper when applicable.

Understanding NIKC's Measurement Tabs Organizational Structure

How do we categorize data?



Our organizational structure enables users to follow nanomaterial transformations while capturing necessary metadata, separating the NIKC database from other nanomaterial databases. To capture the transformations that a nanomaterial may undergo, we sort experimental data into five categories: instance, material, medium, property, and supplementary. Each of the five categories interlace coherently together to catalog the metadata describing the nanomaterial and the exposed medium.

Figure 2. Model of CEINT NIKC measurement structure

The *Instance* is defined as the nanomaterial in a medium at a specific moment in time. We therefore use the Material and Medium category to describe the Instance. In some cases, the Instance will only be defined by the nanomaterial. For example, many times a nanomaterial's initial physical state will be as a powder before it is suspended in solution. In the nanomaterial's powder form, the nanomaterial has no medium. An instance describes the chemical or biological properties of the nanomaterial and the medium at a specific moment in time. A physical or chemical change to the nanomaterial that alters the chemical or biological properties of the medium is described as a new instance.

The *material* is the nanomaterial being studied, whether it exist as a dry powder or dispersed into solution.

The *medium* describes the nanomaterial's environment, which can include the solution that the nanomaterial is dispersed in, the nanomaterial-exposed organism, or organs where the nanomaterial has accumulated.

Properties can be used to describe the medium, material, or supplementary and is where most of the metadata is gathered.

Supplementary are digital data, tables, and documents that cannot be properly interpreted in a numerical or verbal format. TEM images and microscope photos are categorized as supplementary and can associate with material, medium, or property.

Instance

When is there a new instance?

Whenever the material or medium of an instance is so significantly changed that the biological or chemical properties describing the material or medium changes, then the instance is considered to have undergone a transformation resulting in a new instance. Instance changes may include lapses in time such as measurements taken at multiple time intervals. Over time, a nanomaterial may migrate from the exposure point accumulating in one or multiple locations causing a biochemical or immunological reaction, resulting in a new instance. Another example may include functionalization of

the nanomaterial, which changes the chemical properties of the material. A new instance may also be as simple as a physical change from a dry powder to a solution.

Supplementary

How does digital data get stored?

Some data can only be usefully interpreted as visual images, in such cases, verbal descriptions of images are inadequate, and copies of visuals are stored as supplementary data. Supplementary data can include TEM images, histological cross sections, fluorescent images, or diagrams. A property such as diameter or length can have images associated with it. The medium, such as fish or a mesocosm environment also may have a diagram associated with it. Supplementary data can also be flexibly applied to nanomaterials as well.

Property

What does this property belong to?

As stated previously, a property can describe either the material, medium, or supplementary. Salinity or pH are examples of characteristics or properties that describe a solution-type medium. In mammalian test subjects, properties may include age, sex, or weight. Material properties describe the nanomaterial as the nanomaterial transforms. Elemental composition or purity are properties that describe the nanomaterial. Whereas the dose and dose volume describe the material in the exposure medium. Presence of biochemical markers are typically time dependent, material dependent, and medium dependent. Biochemical markers are therefore properties of the medium as the presence of biochemical markers describes the affect a nanomaterial has on the medium at a specific time point.. Supplementary data are generally characterized by the file type, such as jpg or pdf, and the link to the image which we call the filesystem.

Instance Map

Why use an instance map?

An Instance Map is a visual aid that helps a curator to conceptually see how the measurement spreadsheet tabs' organizational structure applies to data curation. Curators who are still learning to define experimental procedures and results as an instance, material, medium, or property, and their relation to each other, will find instance maps useful to refer to during curation. During the nascent

stages of curation, it is helpful to draw out all instances and the materials, media, and properties that define them. Instance Maps are also helpful when curating datasets that test multiple engineered nanomaterials at multiple concentrations where responses are gathered over several time points. An Instance Map should be created before filling out the NIKC spreadsheets to avoid mistakes. Instance maps can help to decrease curation time by helping to eliminate dedicating time to multiple reviews of the article or spreadsheets.

How do I create an instance map?

Preliminary Steps

1. Review your experimental design and associated protocols to identify transformations that have occurred.
 - a. Review what classifies as an instance, material, medium, property, and supplementary, which will make identifying what to highlight easier.
2. Mark every nanomaterial transformation that occurs in the experiments.

Instances- Start with the main roads

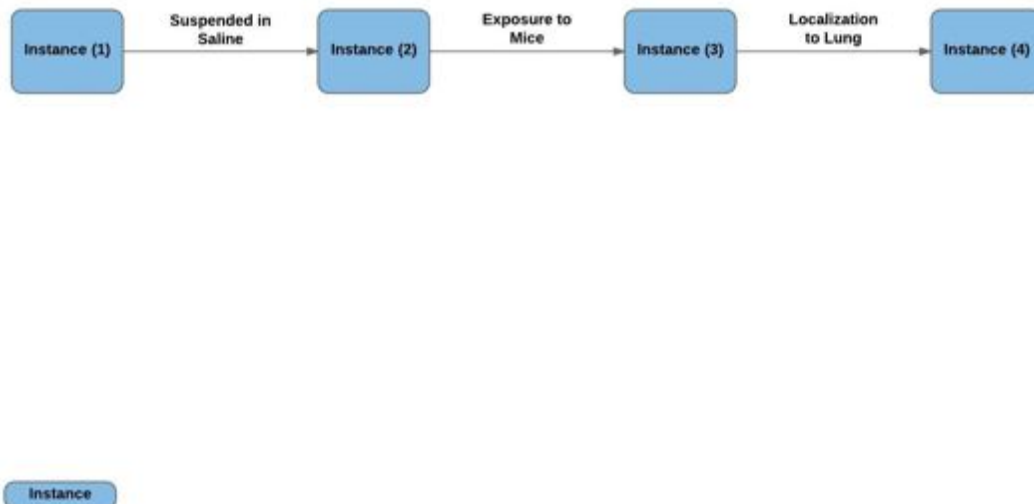


Figure 3. How to draw an instance map: Instances

1. Write each nanomaterial as a separate instance.
 - a. If three nanomaterials are being tested, then three separate instance maps will be created.

- b. A new instance for a nanomaterial should be created if a nanomaterial is functionalized, and both the functionalized and pristine nanomaterial is being tested.
2. Write down every transformation of the nanomaterial as a new instance from its synthesis to its endpoint.
 - a. Remember that an instance is defined by the media, material, and properties at a given moment in time.
3. Draw an arrow between each instance and label the arrow with the transformation that occurred.
 - a. Possible transformations that may occur include changes to the medium or material, and measurement time points.

Materials and Media- Add in side roads

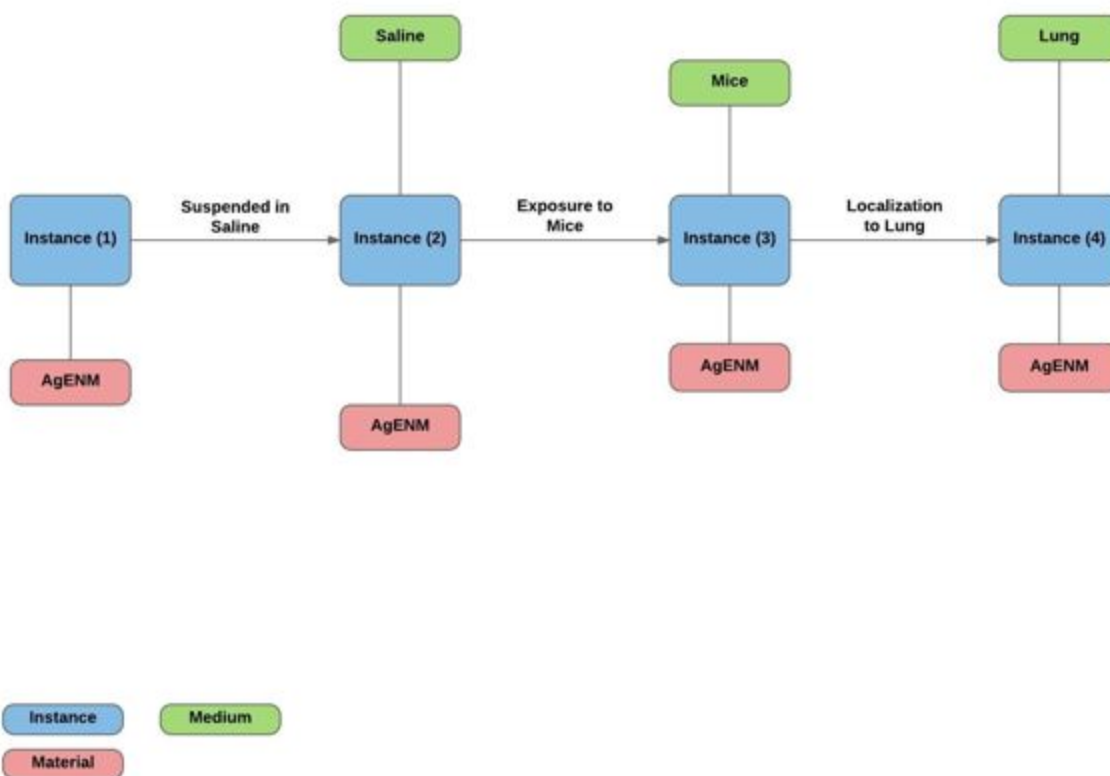


Figure 4. How to draw an instance map: Materials and Media

1. For each instance that you listed, write down the material and medium that defines each one.
 - a. The material and medium can go above or below each instance.

b. Be specific about the labels assigned to the material and medium as these labels will be how you describe the parameter in the spreadsheet.

2. Remember an instance can have more than one medium, but not more than one material.

Properties- What are your destinations?

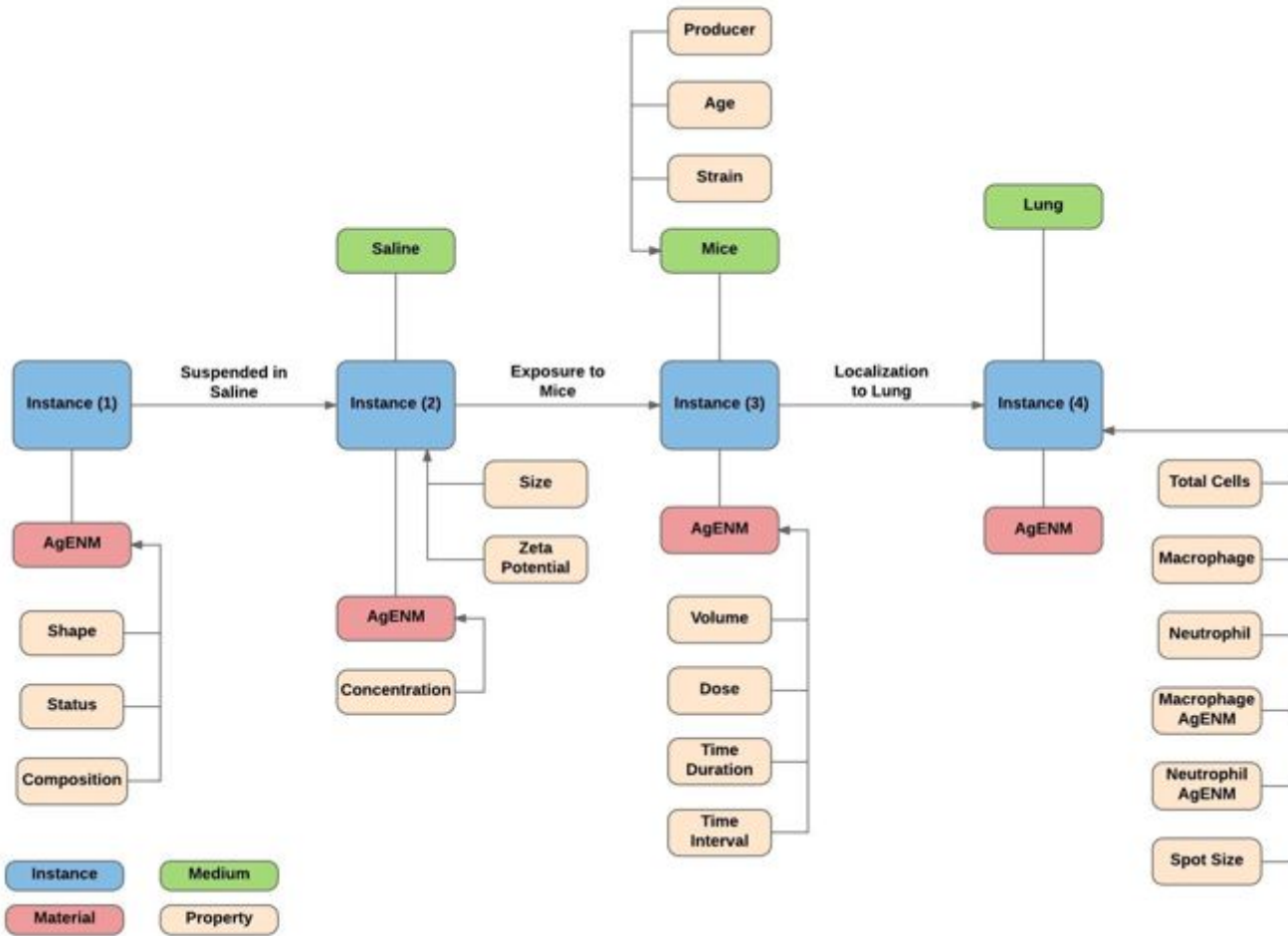


Figure 5. How to draw an instance map: Properties

1. Go back and add in properties to the material and medium.

Supplementary- Any images to show?

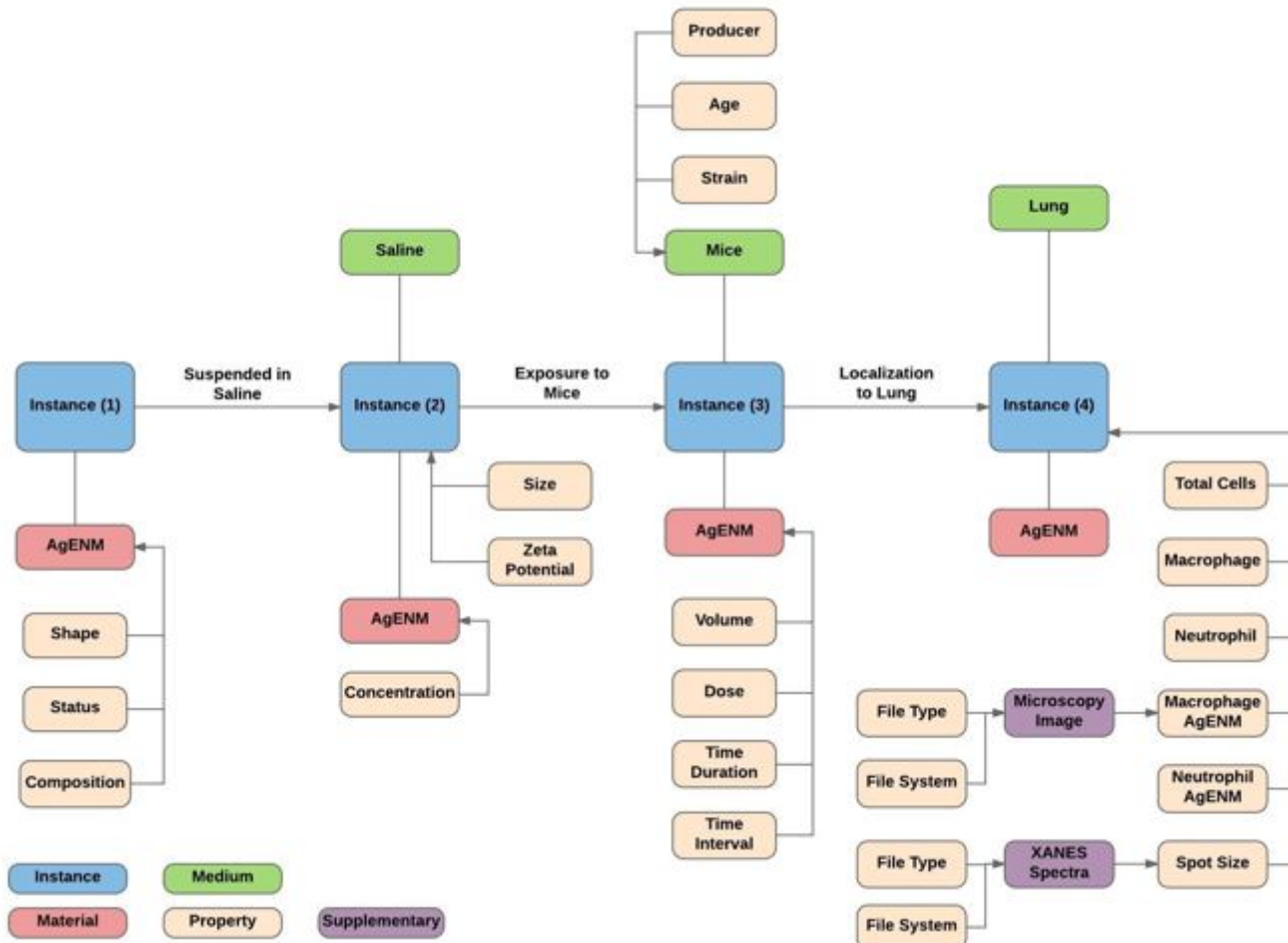


Figure 6. How to draw an instance map: Supplementary

1. Include any images that can be used to describe the material, medium, or measurement.
 - a. Remember to add in properties that describe the supplementary such as the file type.

Step-by-Step Curation and Formatting Guide

How do I curate a paper from start to finish?

What follows is a guide that will help you through every step of curating a dataset, informing you how to fill out every column of every spreadsheet. We suggest that you fill out every column in every row before entering data into the following row. Every person will develop a personal order and process for curation, but we suggest that you start with this guide in the order that it is written until you become familiar with the contents of each spreadsheet and the formatting.

Preliminary Steps

1. Open spreadsheet from template file.
 - a. The same Excel file can be used for repeated experiments with different nanomaterials.
2. If you did not make Instance Map, review your experimental design to identify instances, materials, media, and the properties that describe them.
 - a. The data used to populate the NIKC Excel spreadsheet will come from the NIKC categories that you have identified in your experiment.
 - b. Highlight or mark all information that will be curated from lab notebooks.

Reference Spreadsheets

1. Fill in Publication tab.
 - a. *DatasetID*: Leave blank. The curated dataset will be assigned an ID number by the database.
 - b. *DOI*: Include the DOI if your dataset has been published.
 - c. *Abstract*: If dataset has been published, copy and paste from publication. Your instance map will be included as a visual abstract to accompany your dataset.
 - d. *Keywords*: include words that will help future querying, from a cursory skim. Keywords should be entered into the spreadsheet as follows: [keyword, keyword, keyword].
 - e. *Publish Status*: Published, reviewing, submitted, or preparing.
 - f. *Curation Status*: Mark *Partial*. Update to *Complete* when curation is finished.
 - g. *Curation Note*: Include notes about the curated dataset will provide context for your dataset that was not captured elsewhere in the spreadsheet.

- h. **Embargo Status**: It is incredibly important that you indicate whether or not your dataset can be viewed and used by database users. Input *Yes* or *No* to indicate whether your dataset is embargoed.
- i. *FAIRness*: Leave blank. The database will assign a FAIRness score to your dataset which will indicate how well your curated data adheres to FAIR principles.

Check data format for upload: 1) contactAuthor: Use peopleId, 2) Keywords: must have brackets (e.g. [keyword]).

2. Fill in People tab with one row per researcher.
 - a. If only initials are given, record the initials; however whenever possible record the researcher's full name.
 - b. *People ID* should increase by 1 numerical value with each new researcher.
 - c. Include the name of institution that each researcher is affiliated with in the 'Institution' column in People tab. Only need to include the department if the researcher is associated with more than one department at the same institution.
3. Fill in Institutions tab with all the institutions listed.
 - a. Do not duplicate entries if two or more authors share an institution.
 - b. *Institution ID* should increase by 1 numerical value with each new institution.

Method Spreadsheets

1. For every data point that has a reported protocol in the paper, fill in the Protocol tab.
 - a. *Protocol ID*: Should increase by 1 numerical value with each new protocol. Measurements in Measurement tab will reference this *Protocol ID*.
 - b. *Step ID*: If a protocol has multiple steps, include make each step a new entry. Leave the Protocol ID blank and assign an ID in the *Step Id* column. Should increase by 1.
 - c. *Referencing ID*: For each Step in a protocol reference the *Protocol ID* that the step belongs to, for example, if a Protocol with *Protocol ID 2* has 3 steps, then put the *Protocol ID 2* in the *Referencing ID* column for each step.
 - i. The *Referencing ID* column should only be used protocol steps. Leave the *Referencing ID* column blank for each protocol.

- d. *Name*: If not named directly in paper, give protocol or method a short informative name.
- e. *Duration Value* and *Duration Units*: How long did the protocol last? Do not pluralize units (e.g. hour not hours). Valid values: second, minute, hour, day, week.
- f. *Description*: Describe the protocols or methods used in your experiments.
- g. If there are important parameters within the protocol description text, also add them as properties referenced to the related medium or material. For example: dose, species, age, number of subjects, etc.
- h. *Reference*: List the DOI, ISBN , or website link.

Check data format for upload: *durationUnits* should be singular not plural (e.g. “minute” not “minutes”). DOIs and ISBNs should be formatted brackets (e.g. [DOI, DOI]).

2. For every data point that has a reported instrument in the paper, fill in the *Instrument* tab.
 - a. *Instrument ID* should increase by 1 numerical value with each new instrument. Measurements in *Measurement* tab will reference this *Instrument ID*.
 - b. *Instrument Name*: Type of instrument (e.g. helium pycnometer).
 - c. *Model*: Model name for instrument (e.g. AccuPyc 1340).
 - d. *Manufacturer Name*: Manufacturer of instrument model (e.g. Micromeritics).
 - e. *Manufacturer City, Manufacturer State, Manufacturer Country*: Location where instrument was manufactured.
 - i. No abbreviations. Spell out country’s full name.

Check data format for upload: Make sure every protocol listed and instrument listed in the Protocol Tab and Instrument Tab is attached to a measurement or endpoint in the *Measurement* Tab.

Instance Spreadsheet

1. Compile all of your instances into the *Instance* Tab.
 - a. Dataset ID: Leave blank. Your dataset will be assigned a dataset ID by the database.
 - b. Instance: For instances where the nanomaterial is characterized or a control is run, input stock dispersion, bulk dispersion, or control. For all other instances, assign an Instance ID using the format I0, I1, I2 etc.
 - c. *Time Relative*: How much time has passed since the last instance?

i. If the length of time passed is likely to have influenced the chemistry/biology of the material or medium, then a new instance should be created. E.g. Consider two instances: a rat 24 hours after ingesting nanoparticles, and a rat 48 hours after ingesting nanoparticles. If the 48-hour rat references the 24-hour rat, then *Time Relative* = 24, and *Time Unit* = *hour*.

ii. If the length of time passed is not likely to have influenced the chemistry/biology of the instance, then the property can be related to the same instance.

b. *Time Absolute*: If you know the date that measurements within an instance were taken, include the data here [\(format: needed?\)](#).

Check data format for upload: Units for time should be singular not plural.

Measurement Spreadsheet

Please review "*Understanding NIKC's Measurement Tab Organizational Structure*" section of this manual as needed.

1. Transfer all relevant information from lab notebooks and instruments into spreadsheet.
2. Highlight or mark all transferred information.
3. Fill in the Measurement tab. For each data point:
 - a. *Dataset ID*: Leave blank. Your dataset will be assigned a *dataset ID* by the database.
 - b. *Instance*: Use the list of instance that you have already identified in the Instance tab.
 - c. *Registry Number*: The registry number of your nanomaterial, which can be found here: <https://nanocommons.github.io/identifiers/>
 - d. *Material*: Indicate which nanomaterial you used in your experiment using the appropriate Biomax ID. Biomax IDs can be found here: <https://ssl.biomax.de/nanofase/>
 - e. *Inherit ID*: When an instance has all of the same defining properties of a previous instance, copy the *Instance ID* into the *Inherit ID* column of the new instance.
 - i. When one instance inherits from another instance, it inherits all media, material, properties, and supplementary data of that instance.
 - f. *Medium*: Input the name of the medium where your nanomaterial is located. Remember an instance can have more than one medium. For each medium add a new entry.
 - g. *Measurement Type*: Will always be property

- h. *Parameter*: Name of the data point being recorded.
 - i. This will be the name of the material or medium property (pH, concentration, liver failure rate, etc.).
- i. *Parameter Description*: “Made by experimenter”, “reported by experimenter”, “received from supplier”, “reported by supplier”
- j. *Parameter Data Type*: This will be either “text” or “numeric.” If “text”, also fill in:
 - i. *Parameter Text*: Report the text data (material name, color, species, etc.).
 - 1. Parameter Text for file system should be fs://image/doi_figure_figure number.filetype (e.g. fs://image/10.1016-j.taap.2008.12.006_figure_1.png)
 - ii. If “numeric”, also fill in:
 - iii. *Parameter Statistic*: Statistical descriptors (e.g. mean, mode)
 - iv. *Parameter Numeric*: Report the numeric data (radius, weight, mortality proportion, etc.).
 - v. *Parameter Numeric Operator*: =, >, <, ~.
 - vi. *Parameter Unit*: Units of reported numeric data (centimeter, microgram per liter, dimensionless).
 - 1. Spell it out. No abbreviations.
 - 2. No plural. Gram, not grams.
 - vii. *Parameter Uncertainty Type*: Standard deviation, 95% confidence interval, etc.
 - viii. *Parameter Uncertainty Lower*: Lower value limit of reported measurement.
 - ix. *Parameter Uncertainty Upper*: Upper value limit to reported measurement.
 - x. *Parameter Uncertainty Unit*: Should always be the same as *Parameter Unit*.

Check data format for upload: If you select “text” and input any numerical descriptors, the spreadsheet will not upload onto the database. If select “numeric” and input a text descriptor, the spreadsheet will not upload onto the database. For any “numeric” entry, you must fill in columns: *Parameter Numeric*, *Parameter Numeric Operator*, and *Parameter Unit*.

- k. *Protocol ID*: If applicable, input the appropriate Protocol ID from the Protocol Tab used to take the measurement. More than one protocol ID may be used. Input protocol IDs into the measurement tab in brackets (e.g. [4, 7, 8]). If there is no protocol ID associated with the measurement, leave blank.
- l. *Instrument ID*: If applicable, input the appropriate Instrument ID from the Instrument Tab used to take the measurement. More than one instrument ID may be used. Input instrument IDs into the measurement tab in brackets. If there is no instrument ID associated with the measurement, leave blank
- m. Repeat steps (1-7) for measurement spreadsheet entries from the paper.

Final Steps:

1. Change *Curation Status* in Publication tab to "Complete."
2. Add any thoughts or notes on the publication or data to the *Curation Notes* column of Publication tab (e.g. data that was not curated because it does not fit the scope of the database).