NanoFASE Data Curation Manual

A Visual Guide to Curating Data

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Acknowledgements

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

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The US Center for the Environmental Implications of NanoTechnology (<u>CEINT</u>), The EU projects <u>NanoFASE</u> and <u>NanoCommons</u>, The <u>Labex SERENADE</u> Project.*

^{*}Please see the text-based Manual for names, funding acknowledgements and official disclaimers

Manual Outline

The information contained in this document provide a visual guide for curating NanoFASE data into the EU version of the NIKC template.

This visual curation manual is broken into three parts:

- 1. The EU NIKC Excel Template
- 2. How to create the Instance Map
- 3. Translating the map to Template







NanoFASE 2 NIKC Curation Process

3 **Initiating Steps** NanoFASE R NIKC Correct any Fill NanoFASE Customize **Review curation** Generate **Curation Manual** errors in NanoFASE Excel **Excel Template** instance manual and Shared dataset and with Dataset(s) **Template** map as a note any send to Curator Meeting (columns, visual questions Schedule Set curator abstract* parameters) ~1.5 hours ~24 hours * ~2 hours ~4-5 hours* Review with Review with Review with Review with curator to curator to curator to curator to resolution. resolution. resolution. resolution. ~0.5 hour Curator ~2 hours ~1 hour ~16 hours **UPLOAD** *Depends on size of dataset * This step may be moved to the end if the data owner prefers to work in the Excel template first







Part 1: The EU NIKC Excel Template

The first section of the visual manual goes through every column of every Excel tab, while also providing information on how the spreadsheets are connected together.

It explains what information should captured where, while providing a list of 'valid values' for input into columns.

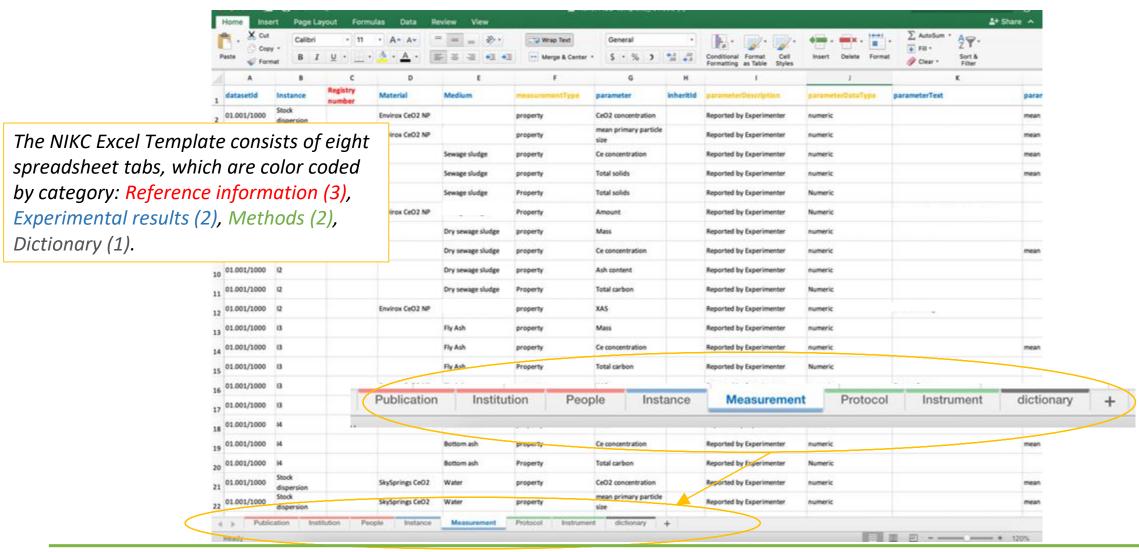
The goal for curating into the level of depth necessary for the NIKC is to capture all necessary metadata for experiments to be replicable and further analyzed.







Navigating the NanoFASE Curation Process: Curation Excel









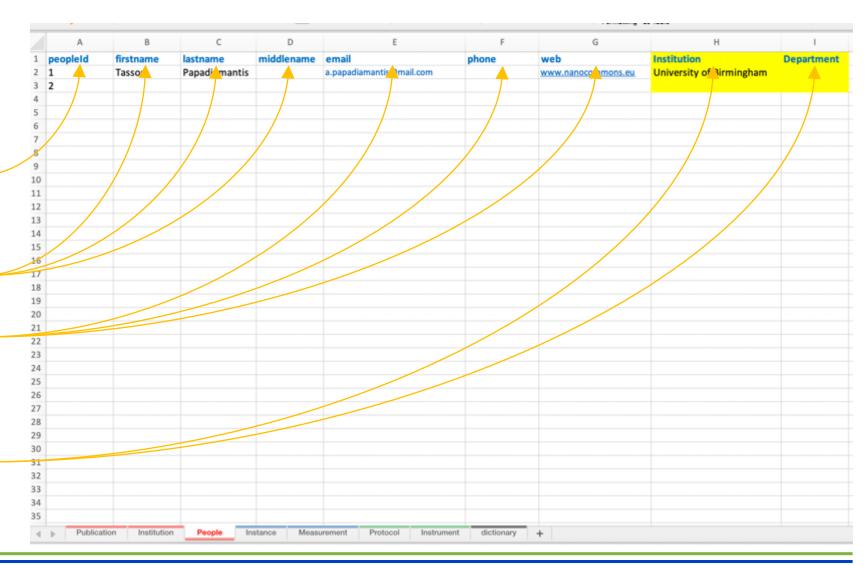
The "People" tab is where we record who worked on the study.

Give each person in the study a unique ID in order 1, 2, 3 etc..
The database will assign truly unique IDs during the upload process.

Input person's name.

Input person's contact information.

Input the name of the institution. *Include the department on the people tab only if data submitters come from the same institute but different departments





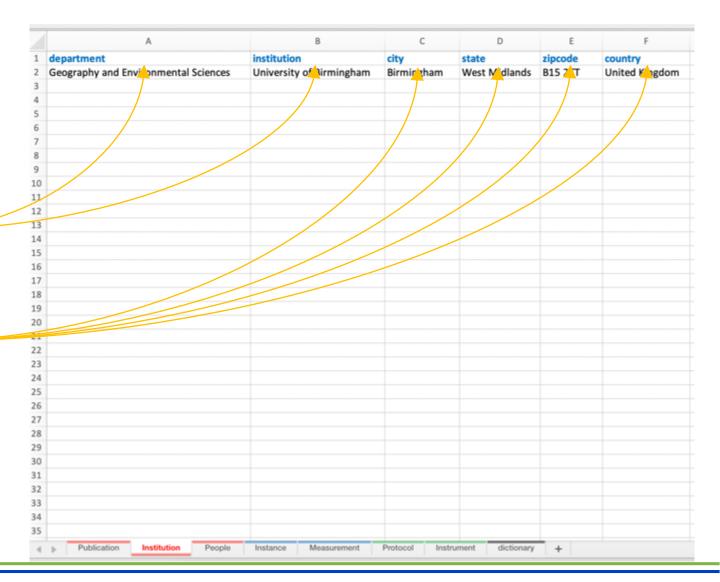




The "Institution" tab is where we record the study's associated institutions.

Input the name of the institution(s) and the associated department.

Input where the institution(s) is located.









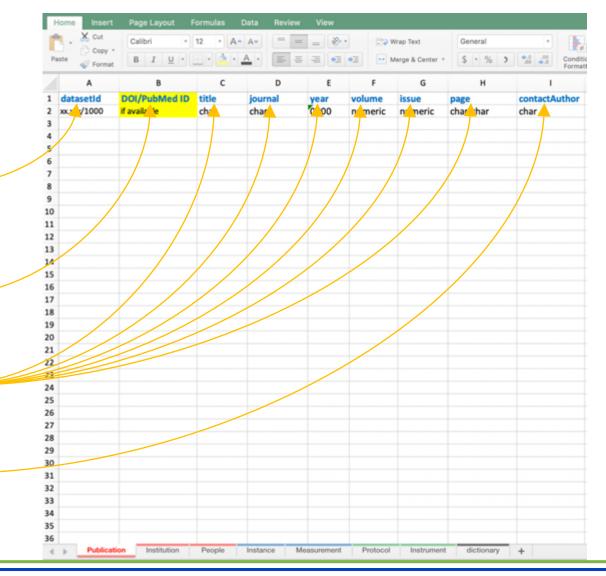
The "Publication" tab is where we record the bibliography information of published studies (Column A – I).

The datasetId will be assigned by the database. Leave blank for now.

Use the DOI of the publication if the dataset has been published.

Input article referencing information.

Input who is listed as the contact author for the publication.









The "Publication" tab is where we record the bibliography information of published studies (Column J – P).

Input keywords that describe the publication.

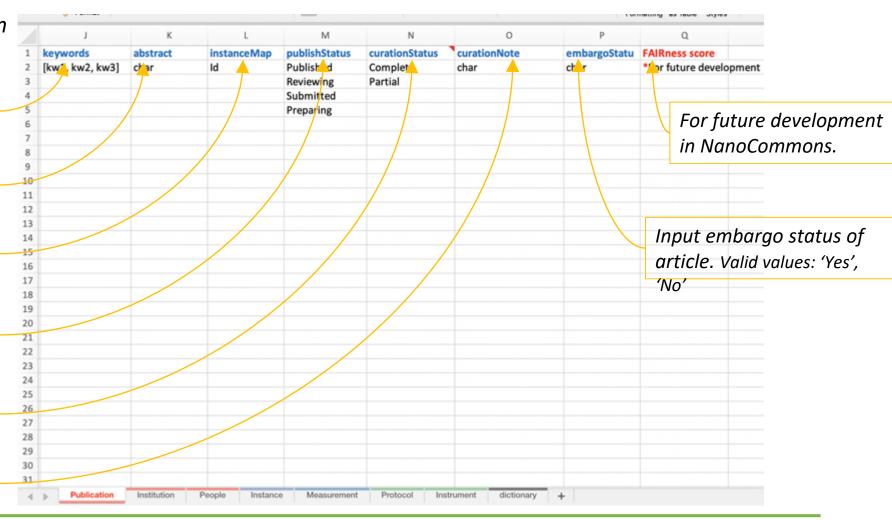
Input the entire abstract from the publication.

The datasetId will be assigned to your Instance Map.

Input publication status of article. Valid values: 'published', 'reviewing', 'submitted', 'preparing'

Input curation status of article. Valid values: 'complete', 'partial'

Input any curation notes. E.g. Not all figures curated.









The "Protocol" tab is where we record the experimental designs and protocols used to take measurements and endpoints recorded in the study. (Column A-F)

Give each protocol an unique ID. A number that has not already been assigned to another protocol.

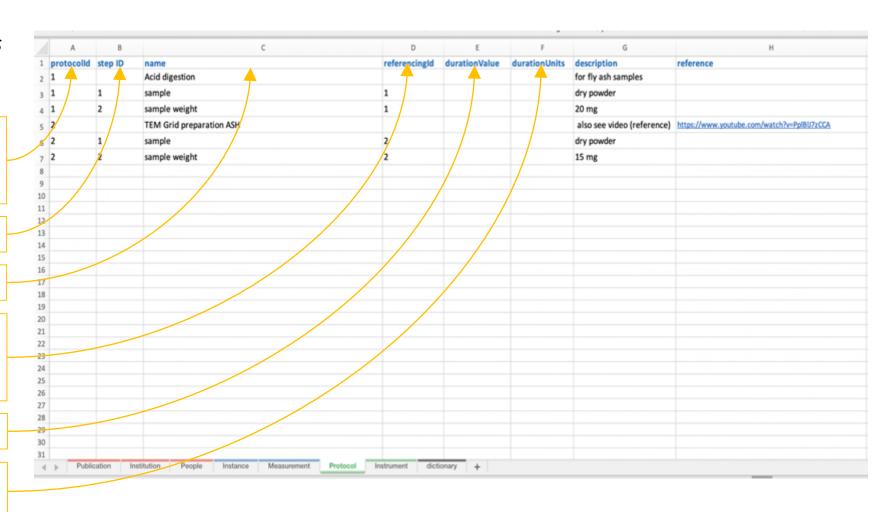
Give each step in a protocol an unique ID.

Input the name of the protocol or step.

For each protocol step, put the "protocolld" of the protocol that the step belongs to.

Input how long the protocol last.

Input time units. Valid values: 'second', 'minute', 'hour', 'day', 'hour', 'week', 'month'





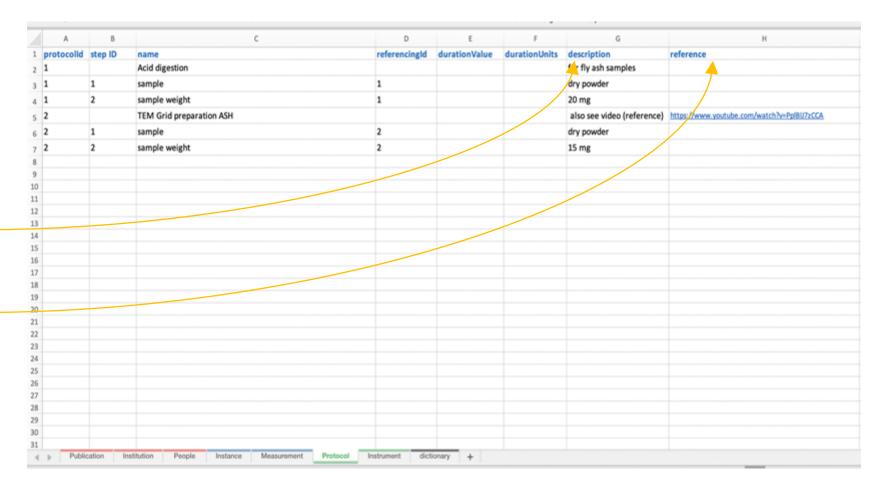




The "Protocol" tab is where we record the experimental designs and protocols used to take measurements and endpoints recorded in the study. (Column G-H)

Describe the method or protocol used.

Input any references for the method. Valid values: DOIs, ISBNs, website links









The "Instrument" tab is where we record the instruments used to take measurements and endpoints recorded in the study.

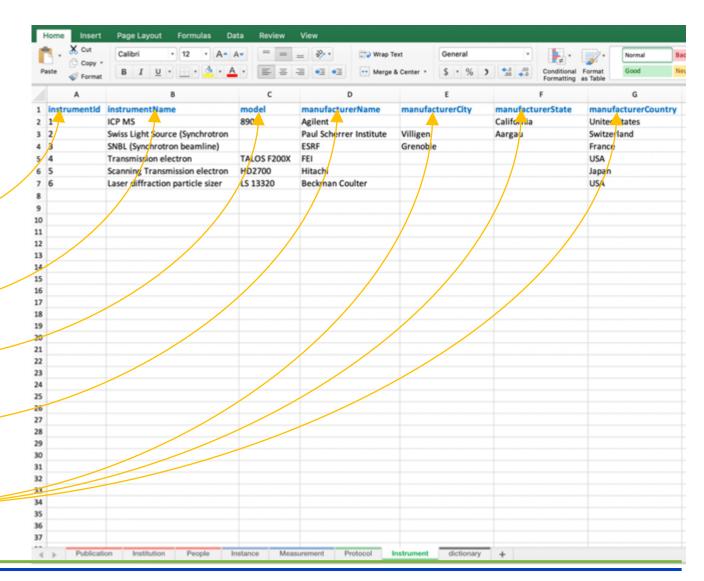
Give each instrument an unique ID. A number that has not already been assigned to another instrument.

Input the name of the instrument.

Input the model of the instrument.

Input the name of instrument's manufacturer.

Input where the manufacturer is located.









The "Instance" tab is where we record the time parameters describing all the instances in a given study.

The datasetId will be assigned by the database.

Give each Instance row a unique numerical ID in the order they occur in your experiment, except for Instances where the nanomaterial is characterized or a control is run. When the nanomaterial is characterized or a control is run input: valid values: 'stock dispersion', 'bulk dispersion', 'control', or 'solid material'.

Input the amount time that has passed since the last set of measurements or specific reference point (e.g. post plant emergence). Start with time 0.

Input the time unit relevant to your experiment. This can be simple time units (e.g. day, hour) or more specific (e.g. day post fertilization)

datasetId	Instance	timeRelative	timeUnit	timeAbsolute	timeUnit	Date
01.001/1000	Stock	o	Day	0	Day	22-Dec-18
01.001/1000	Bulk dispersion	0	Day	0	Day	
01.001/1000	Coating control	0	Day	0	Day	
01.001/1000	Control	9	Day	0	Day	
01.001/1000	10	0	D ay	0	Day	
01.001/1000	l1 /	7	Day	7	Day	
01.001/1000	12	1	Day post emergence	8	Day	
01.001/1000	13	4	Day post emergence	11	Day	
01.001/1000	14	6	Day post emergence	13	Day	
01.001/1000	15	13	Day post emergence		Day	
01.001/1000	16	27	Day post emergence	34	Day	
01.001/1000	17	0	Day		Day	







The "Instance" tab is where we record the time parameters describing all the instances in a given study.

Input the actual time that has passed since you started the experiment.

Input the time unit. This can only be a simple time unit (e.g. sec, min, hour, day, hour, month).

Input the date and time of measurement, if possible.

datasetId	Instance	timeRelative	timeUnit	timeAbsolute	timeUnit	Date
01.001/1000	Stock dispersion	0	Day	0	Day	22-Dec-18
01.001/1000	Bulk dispersion	0	Day	0	Day	
01.001/1000	Coating control	0	Day	0	Day	
01.001/1000	Control	0	Day	0	Day	
01.001/1000	10	0	Day	0	Day	
01.001/1000	!1	7	Day	7	Day	
01.001/1000	12	1	Day post emergence	8	Day	
01.001/1000	13	4	Day post emergence	11	Day	
01.001/1000	14	6	Day post emergence	13	Day	
01.001/1000	15	13	Day post emergence		Day	
01.001/1000	16	27	Day post emergence	34	Day	
01.001/1000	17	0	Day		Day	







The "Measurement" tab is where we record the measurements and endpoints recorded in the study. It is where we link the reference and methods tabs together, and instances to defining parameters such as the material or medium. (Column A - F)

The datasetId will be assigned by the database.

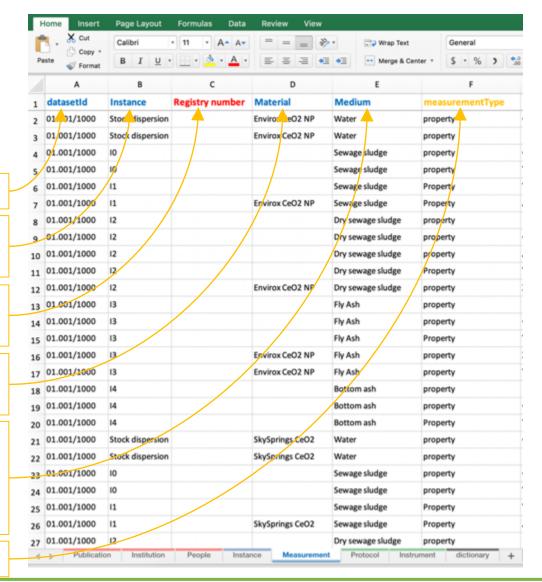
Link instances from "Instance" tab to measurement tab using Ids.

Include registry number of nanomaterials from the NanoCommons's project. See next slide

Input the material name using the BiomaxID given to each unique nanomaterial. See next slide

Input the medium or environment that the nanomaterial is in. Keep in mind this could be an environmental medium, or an animal, or any surroundings.

The "measurementType" should always be property.

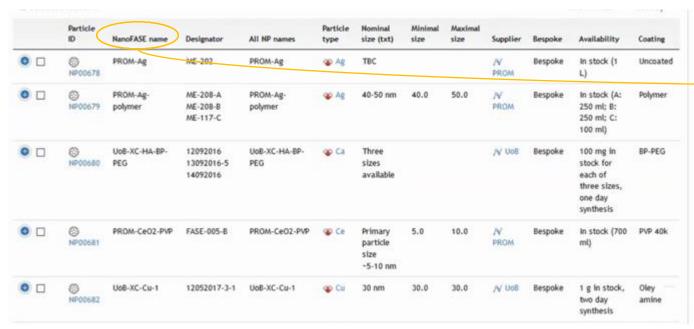








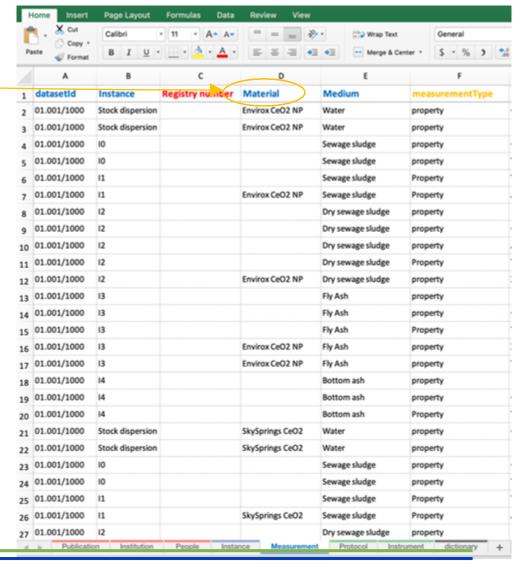
Measurement Tab: Naming the Material





The NanoFASE Knowledge Base assigns an unique Id to nanomaterials used in the project. The link above will allow you to search the Knowledge Base to find the nanomaterial you used in your experiment. Input the name of your nanomaterial found in 'NanoFASE name' column, in the 'Material' column of the Excel template.

*Note: you will need a username and password to access. Contact: nanofase@biomax.com









Measurement Tab: Naming the Material

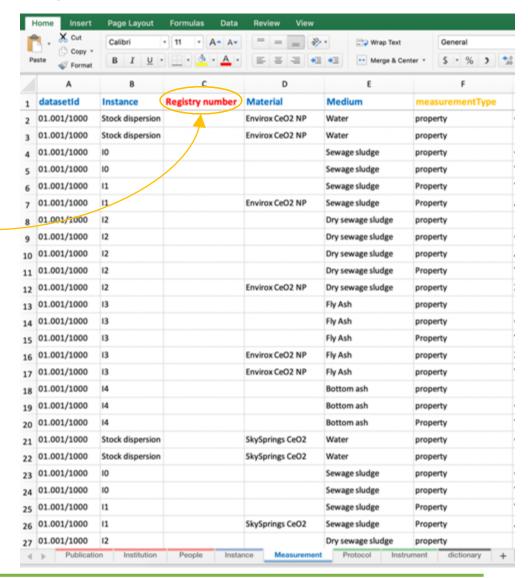
"The European Registry of Materials is a simple registry with the sole purpose to mint material identifiers to be used by research projects throughout the life cycle of their project.

The Registry has been initiated by the NanoCommons project by Maastricht University and is been supported by CEH and UoB.

All NanoFASE materials will be added into the registry and linked to both the NanoFASE portal and submitted datasets in the highlighted column

This is a process that has been assigned to UoB and CEH and will take place during the duration of the NanoCommons project and will continue after NanoFASE has ended.

NanoFASE partners are free to register the materials they used, if they wish, but this is not mandatory for the data capturing process. If you would like to do so see the next slide, visit the registry online via the link provided to start the registration process. Else please skip to slide 19.









Measurement Tab: Naming the Material

How to register new materials

The process to register new materials is described in this document.

How to use the identifier

The identifier is supposed to be use in all written material. The identifier will be a simple identifier starting with "ERM". It is recommended to use the identifier in the Compact Identifier form (identifiers.org entry)

Use in semantic web solutions

For use in semantic web approaches, an equivalent IRI version is available with prefixes the short identifier with "https://nanocommons.github.io/identifiers/registry#".

Registered materials

- . the full list can be found at https://nanocommons.github.io/identifiers/registry Prurtle format)
- ERM00000001-ERM00000057 for NanoSolvel7
- · < you can be the second >

Acknowledgement

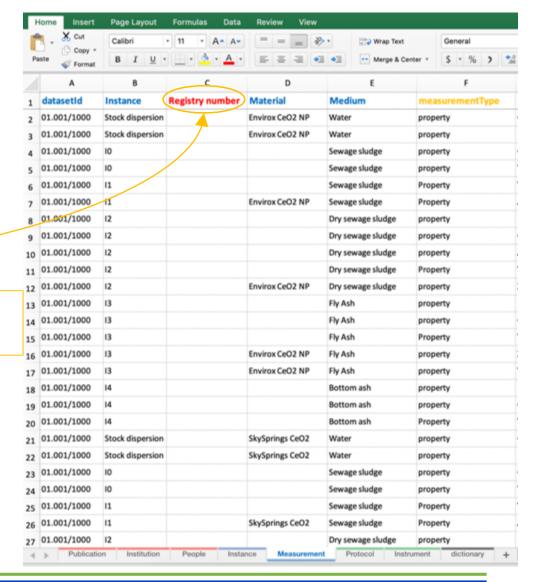
Select the highlighted link to access the list of registered materials.

This registry is supported by NanoCommons. NanoCommons has received funding from European Union Horizon 2020 Programme (H2020) under grant agreement no 731032.



https://nanocommons.github.io/identifiers/

"The European Registry of Materials is a simple registry with the sole purpose to mint material identifiers to be used by research projects throughout the life cycle of their project (From above website)." Input the registry number of the nanomaterial found in the downloaded document, in the 'Registry number' column of the Excel template.









The "Measurement" tab is where we record the measurements and endpoints recorded in the study. It is where we link the reference and methods tabs together, and instances to defining parameters such as the material or medium. (Column G - K)

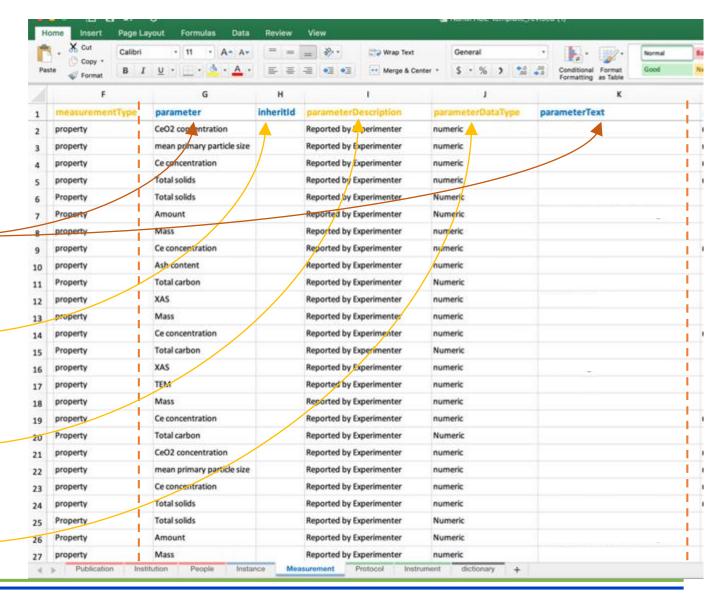
Input the measured parameters/endpoints.

Only input parameterText values if the measurement is not numerical.

If parameter values are the same from a previous 'instance', then input the InstanceId here.

Input who made or recorded the measurement. Valid Values: 'Made by Experimenter', 'Reported by Experimenter', 'Received from Supplier', 'Reported by Supplier', 'Reported by Modeler'

Input whether the parameter is in a text or numerical format. Valid Values: 'Text', 'Numeric'









The "Measurement" tab is where we record the measurements and endpoints recorded in the study. It is where we link the reference and methods tabs together, and instances to defining parameters such as the material or medium. (Column L - T)

Input statistic qualifier of numerical value. Valid values include: 'mean', 'median'

Input number of samples.

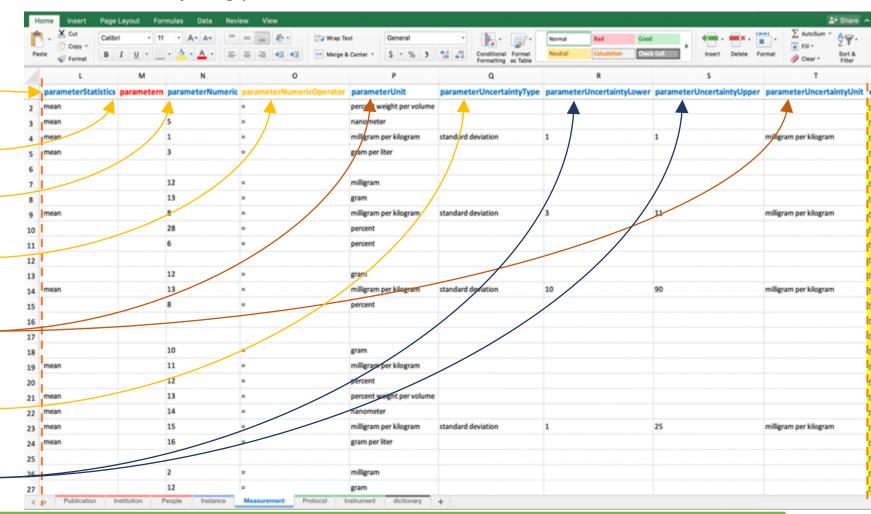
Input the numeric value.

Input operator qualifier of numerical value. Valid values include: '<', '>', '=', '~'

Input unit describing numerical value (in singular form e.g. milligram not milligrams).

Input numerical uncertainty. Valid values include: 'standard deviation', 'range', 'standard error of the mean', 'standard error'

Input numerical values of uncertainty.









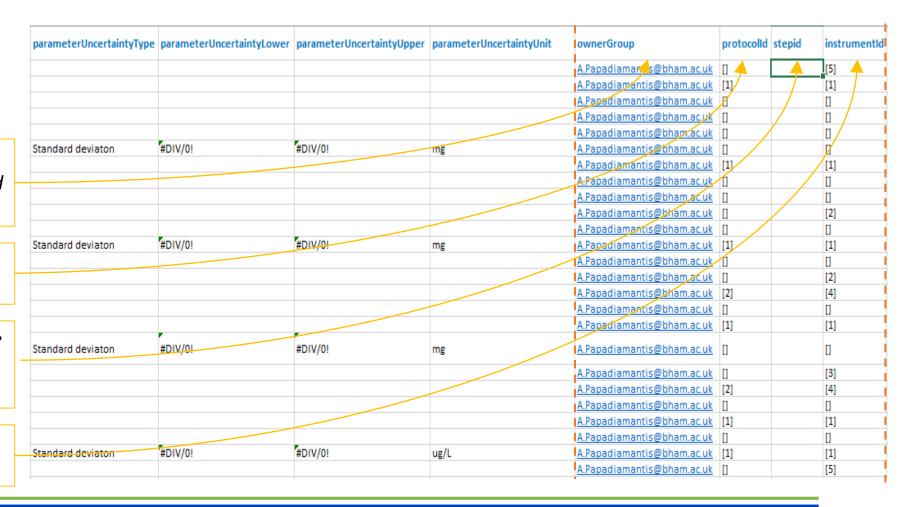
The "Measurement" tab is where we record the measurements and endpoints recorded in the study. It is where we link the reference and methods tabs together, and instances to defining parameters such as the material or medium. (Column U – W)

Input the email for who measured the endpoints and characterizations recorded in the spreadsheet.

Input the protocolld of the method used to take a measurement or endpoint.

Input the stepId of the protocol used take a measurement or endpoint. Include if your protocol has multiple steps.

Input the instrumentId of the instrument used to take a measurement of endpoint.







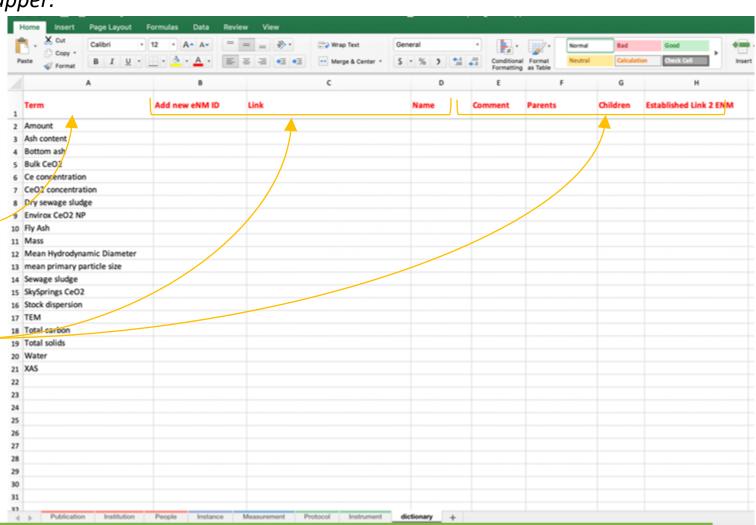


Navigating the NanoFASE Curation Process: Dictionary Tab

The "Dictionary" tab is where we record the all of the parameter and parameterText terms recorded in the study. It is where we link to outside ontologies such as eNanoMapper.

Add the key terms that you believe would be critical in designing queries to find datasets similar to yours.

Leave columns blank. These columns will be filled out by the curator









Part 2: How to Create the Instance Map

The second section of the visual manual delves into how to make your Instance Map(s), which is a visual representation of your experiment(s) applying NIKC database concepts.

Your Instance Map will be uploaded onto the database to accompany your dataset.

When users are querying the database to determine if your dataset will be useful for their needs, your Instance Map will quickly communicate experimental parameters and designs.







NIKC Curation: Categorizing Data

Instance

Describes the chemical or biological properties of the nanomaterial and the medium at a specific moment in time.

Material

The nanomaterial being studied.

Medium

Describes the nanomaterial's environment(s).

Supplementary

Digital images, documents, or tables.

Property

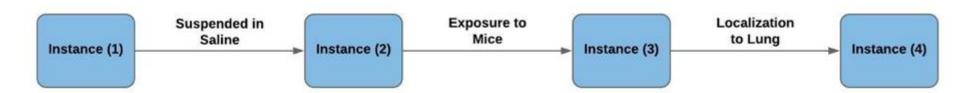
Can be used to describe the instance, medium, material, or supplementary.







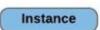
Step 1: Identify Your Instances



How do I identify my Instances?

Has a change occurred that transformed the properties of the nanomaterial or the medium?

- Functionalization of the nanomaterial
- Dispersion of the nanomaterial in solution
- Time point measurements
- Transport/Accumulation of the nanomaterial from the exposure site



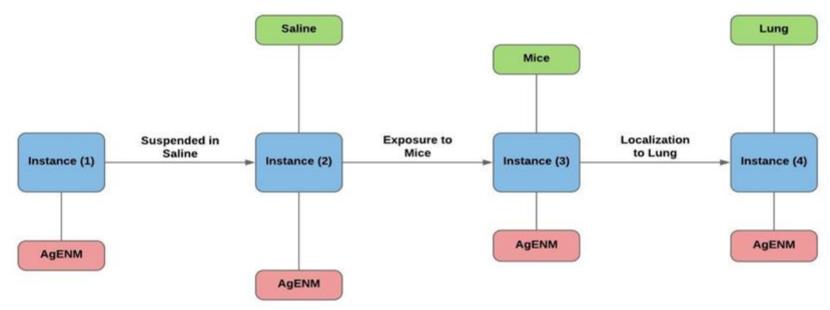
Describes the chemical or biological properties of the nanomaterial and the medium at a specific moment in time.







Step 2: Identify Materials and Mediums



Rules for the Medium and the Material

- An Instance can have more than one medium
- Each Instance Map can only have one nanomaterial. If there is more than one material for an experiment, then another instance map needs to be created.



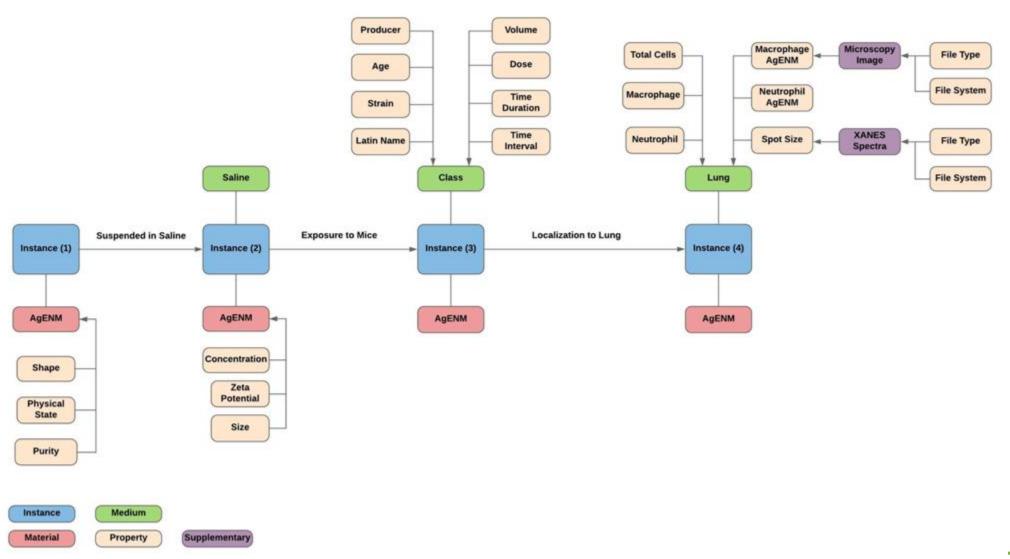
Smulders, S et al. Toxicol Lett 238 (1), 1-6. 2015 Oct 1.







Step 3: Measurements and Endpoints









Part 3: Translating Your Map to Template

The third section of the visual manual delves into how to translate your Instance Map to the Excel template, connecting the template your NIKC adapted experiment.

The translation section will walk you through where to put the information from map in the template.

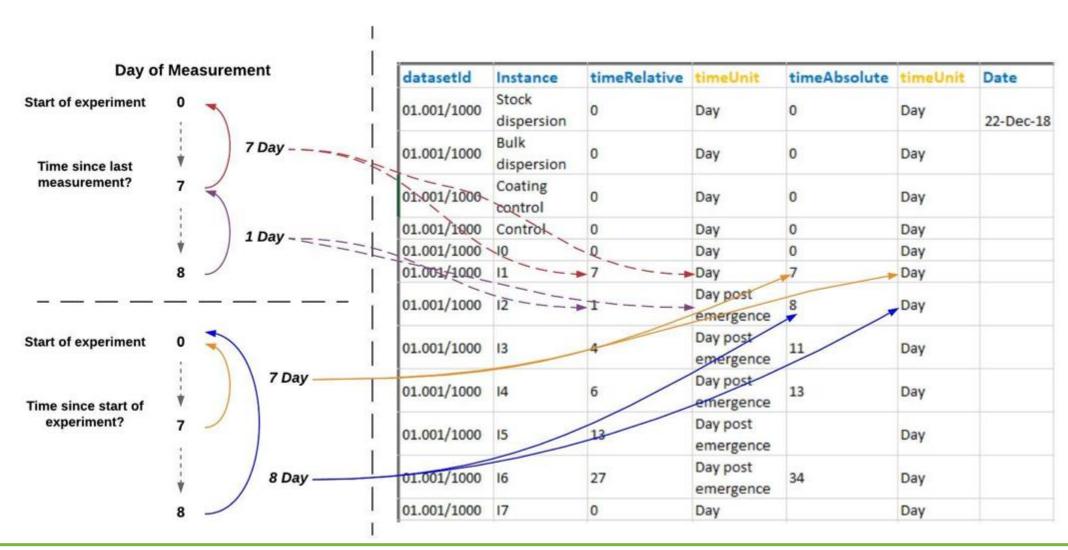
You can think of your Instance Map as the blueprint for how you will layout your Excel template.







Time-Dependent Measurements

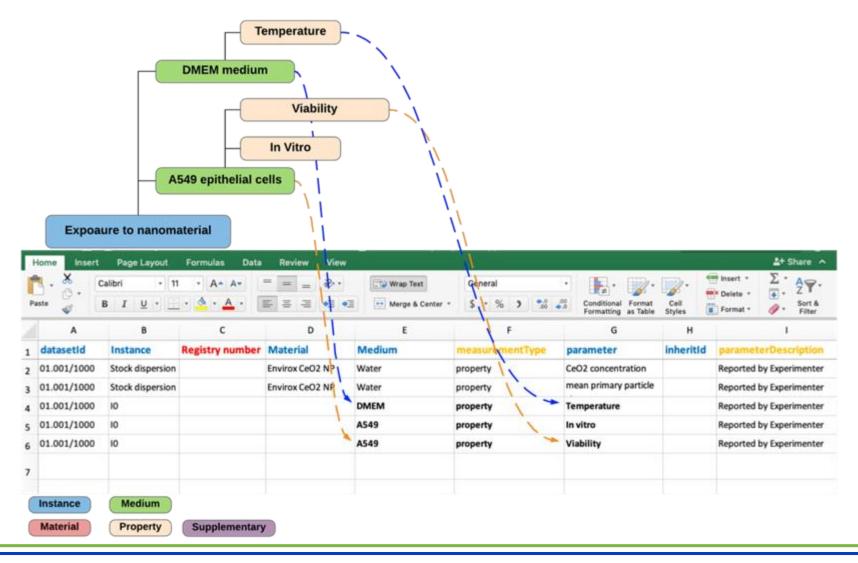








Identifying Parameters: Medium









Additional Help Sources

- If you are in need of additional information, please refer to:
 - Example Excel Template: This template provides example diagrams explaining how to fill out the Excel Sheets.
 - Curation Word Manual: The Word document provides more explanations on the NIKC concepts and NIKC Excel Template discussed in visual manual.
- Please submit completed curated templates by:
 - Initial datasets to be submitted by end of August and uploaded for the final review meeting
 - All datasets by 20 September 2019
 - All to be sent to Anastasios Papadiamantis (A.Papadiamantis@bham.ac.uk)





