ACEnano
Analytical and Characterisation Excellence

NanoCommons
Nano-Knowledge Community

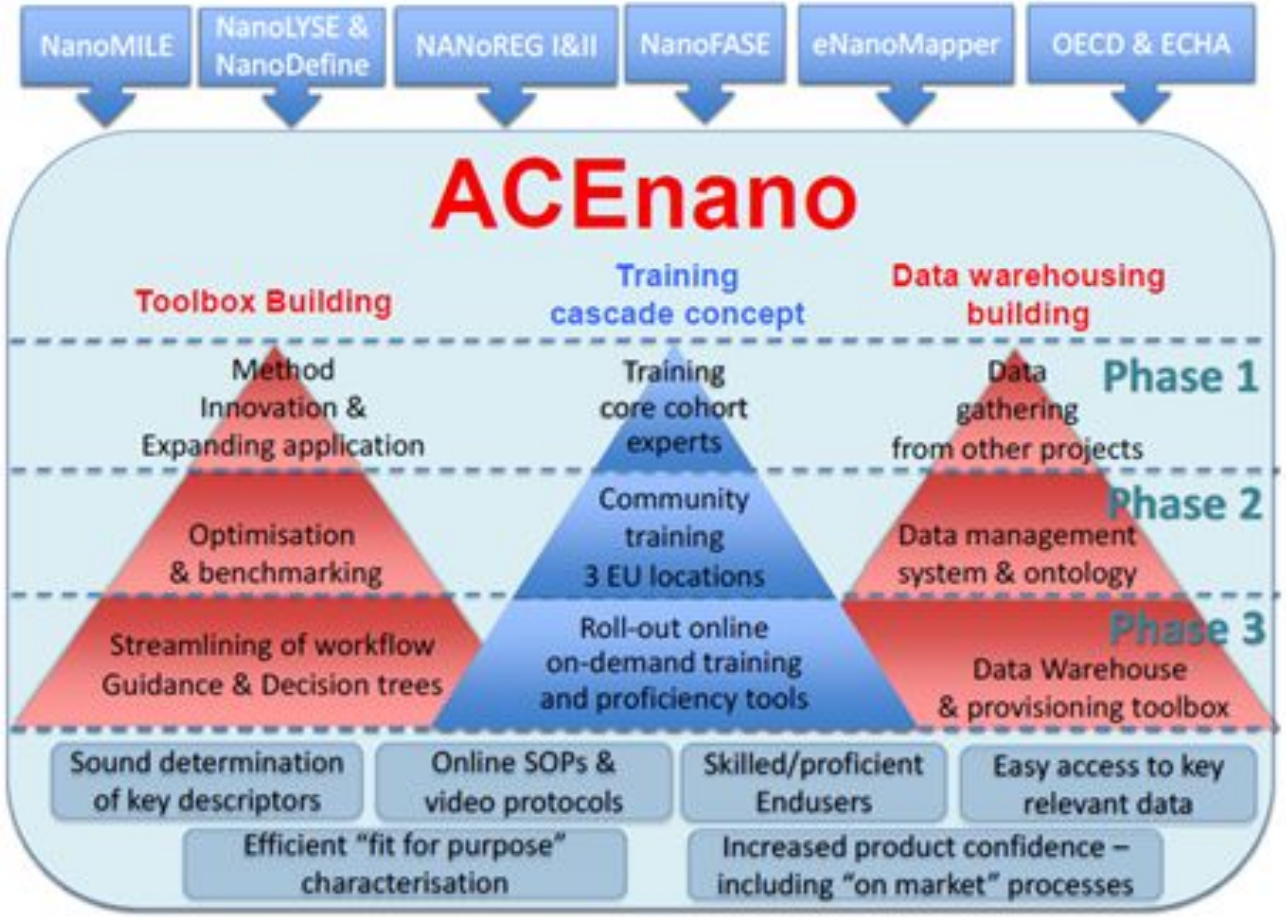
ACEnano
Analytical and Characterisation Excellence

ACEnano knowledge infrastructure to support data collection, methods optimisation and knowledge sharing in the area of physicochemical characterisation of nanomaterials

Thomas Exner, Edelweiss Connect (Switzerland)

NanoSafety Cluster week
09 October 2019, Copenhagen, Denmark

Analytical and Characterisation Excellence in nanomaterial risk assessment: A tiered approach



A tiered approach

ACEnano (Horizon 2020; Project number 720952) aims to introduce confidence, adaptability and clarity into nanomaterial risk assessment by developing a widely implementable and robust tiered approach to **nanomaterials physicochemical characterisation**.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 720952

www.acenano-project.eu

ACEnano

Analytical and Characterisation Excellence

Analytical and Characterisation Excellence in nanomaterial risk assessment: A tiered approach

ACEnano will introduce **confidence, adaptability and clarity into nanomaterial risk assessment** by developing a widely implementable and robust tiered approach to nanomaterials physicochemical characterisation

Main outcome: ACENANO TOOLBOX, available online and comprising:

- Analytical **innovation** in non-existent or poorly developed techniques
- **Optimisation** in existing techniques/instrumentation
- **Benchmarking/standardisation** in well developed techniques
- Three layer **training** model: core cohort of experts from the consortium, community training events, and online training tools
- **Decision tree** to guide users (specially SMEs) through selection of the most appropriate methods to address their needs in risk assessment

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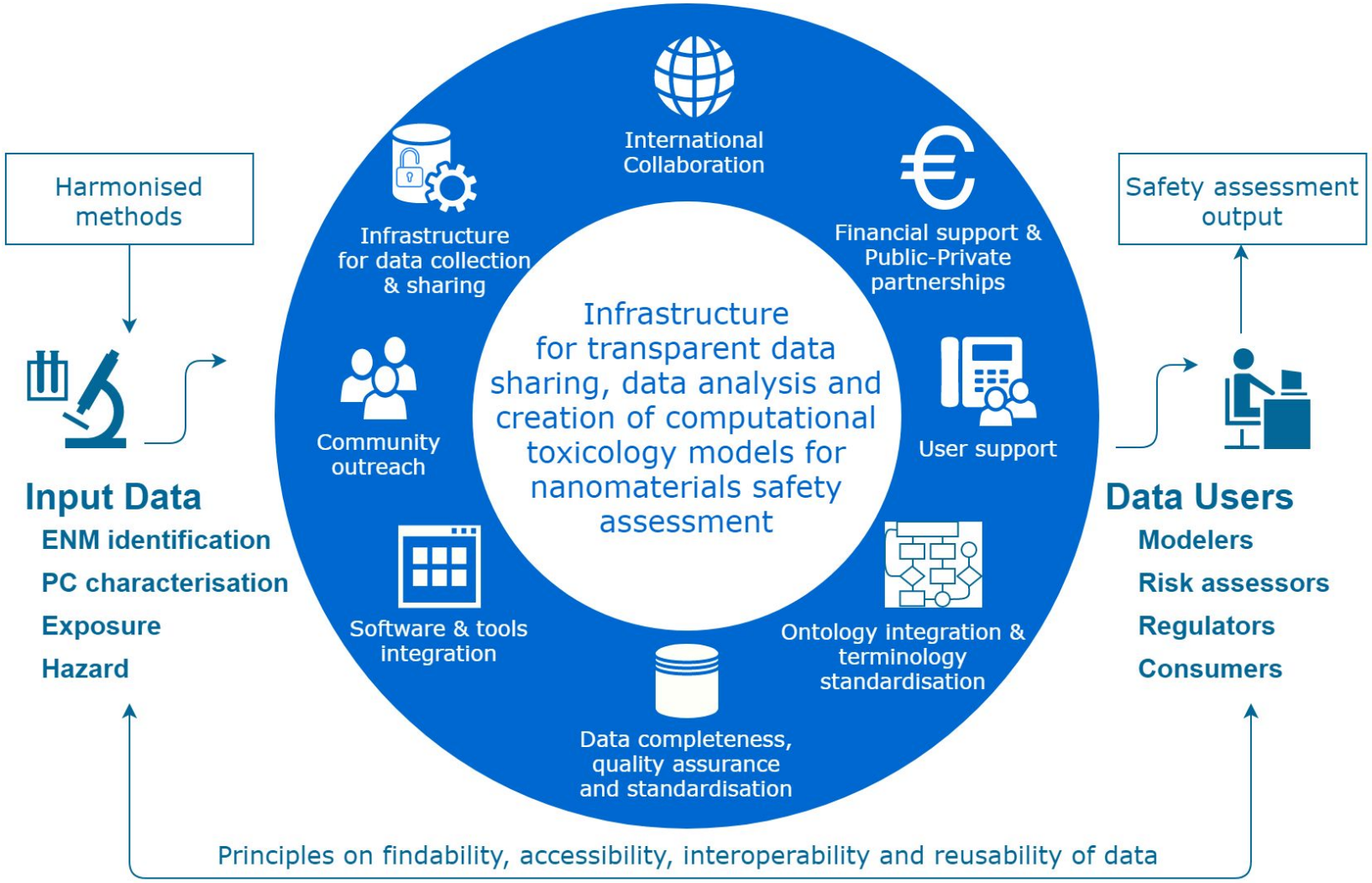
Knowledge warehousing

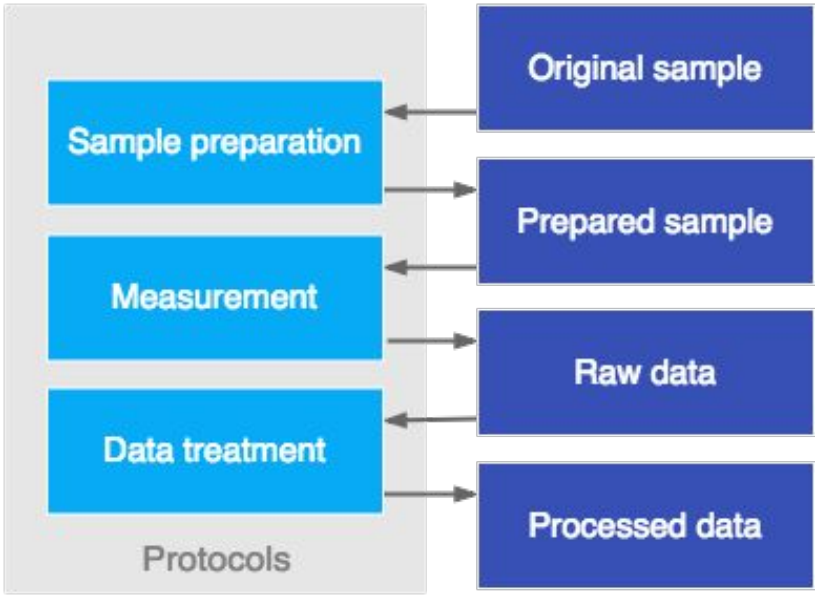


Fadeel B, Farcal L, Hardy B, Vázquez-Campos S, Hristozov D, Marcomini A, Lynch I, Valsami-Jones E, Alenius H, Savolainen K, Advanced tools for the safety assessment of nanomaterials, *Nature Nanotechnology 13, 537–543 (2018),* DOI: 10.1038/s41565-018-0185-0

Knowledge warehousing

Protocols

- Access and sharing of methods
- Collection of metadata on the experimental procedure
- Tracking details on the steps performed
- Linked the method with the result
- Comparison of the experimental design
- Searchable and easy to filter database



Data

- Selection and use any of the methods added in the protocols database
- Create and save the full workflow applied
- Support intra- and inter-laboratory reproducibility goal
- Document all steps performed on a sample from the identification to the final characterisation results
- Storage and sharing of data

Why did we decide on a new concept?

ACEnano tasks are:

1. Develop new and optimize existing characterization methods
2. Round robin testing for interlaboratory testing
3. Standardization of methods

Solution: Covering exact details as computer-readable metadata able to show even small differences in form of a questionnaire.

Protocols

Sample preparation protocol	
Part 1: General information	Protocol name and description
	Contacts
	Technique and Endpoints
Part 2: Steps	Multiple actions and action parameters
→ **Preview protocol, Make more changes & Submit protocol**	

Data treatment protocol	
Part 1: General information	Protocol name and description
	Contacts
	Technique and Endpoints
Part 2: Steps	Steps and algorithm used
→ **Preview protocol, Make more changes & Submit protocol**	

Measurement protocol	
Part 1: General information	Protocol name and description
	Contacts
	Technique and Endpoints
Part 2: Equipment	Instrument settings
	Type of datasets produced
	Measurement quality parameters
Part 3: Steps	Protocol steps
→ **Preview protocol, Make more changes & Submit protocol**	

Protocols: measurement

Part 2: Equipment

Equipment

Please describe the equipment used to preform the measurement. Be sure to provide details on any instrument settings that may introduce artefacts in the final result.

Name:*

Model:

Common instrument makes and models.

Instrument type:

Software:

Software version:

Limit of detection upper:

What is the largest value of the endpoint that can be measured? If there are no definite detection limits please mention the particle or medium properties that limits the detectability as a function of size.

Limit of detection lower:

What is the lowest value of the endpoint that can be measured?

Limit of detection unit:

Instrument settings and parameters (optional)

List instrument settings and parameters that might influence the measured value or its accuracy, or are of importance for reproducing the experiment. Where applicable, also give units of these settings.

Setting	Value	Unit	
Setting	Value	Unit	delete
Setting	Value	Unit	delete
Setting	Value	Unit	delete

Possible datasets

State the type and units of each of the axes of raw data that can be produced by your instrument that are pertinent to the endpoint in question.

Axe:* **Units:** Delete

+ Add another axe

Measurement quality parameters

State parameters that are measured by the instrument that give an indication of the accuracy or validity of the endpoint. State also their units if applicable.

Parameter:* **Common setting:** **Units:** Delete

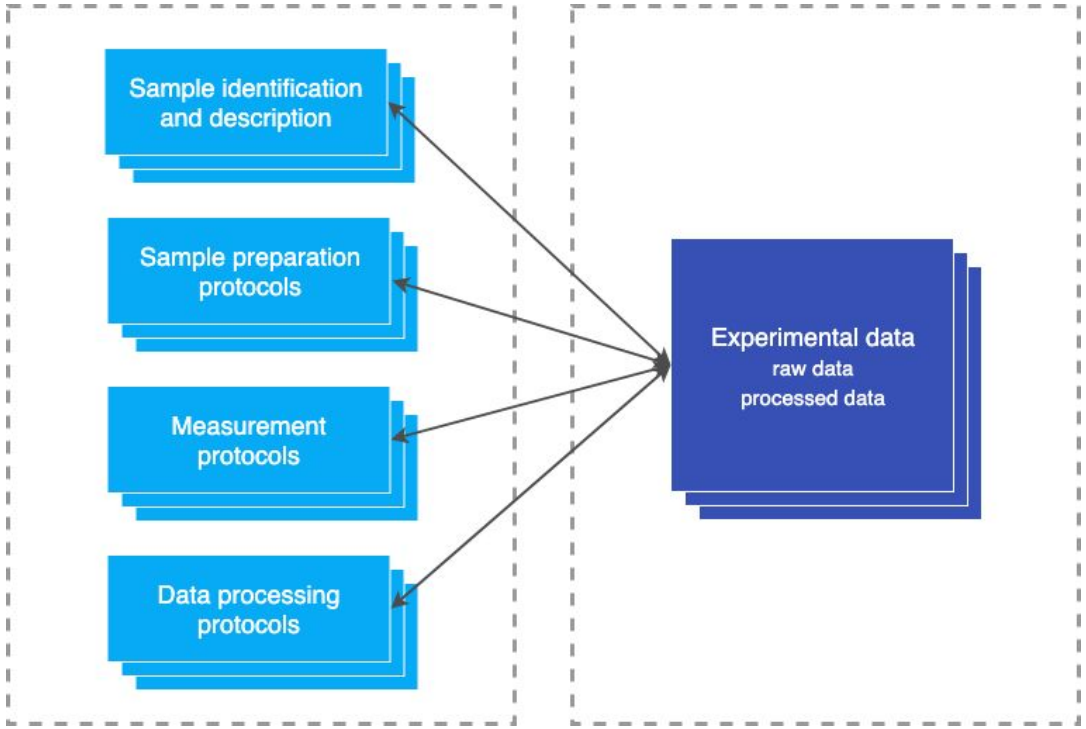
+ Add another quality parameter

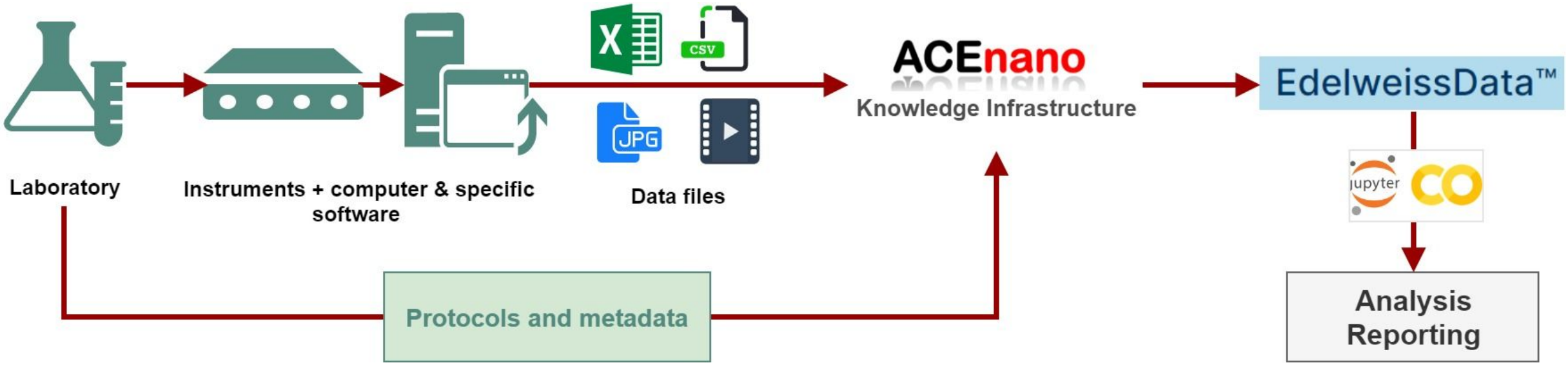
Continue to next step

Data

Data upload process:

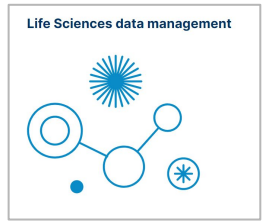
1. Select the technique used in the analysis and which endpoints were measured.
2. Select which sample preparation protocol was used.
3. Select the measurement protocol.
4. Select which data treatment protocol was used.
5. Provide details such as analysis name, description, and contact information.
6. Provide description of the sample that was used in the measurement.
7. Upload raw and processed data files.

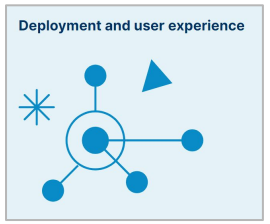


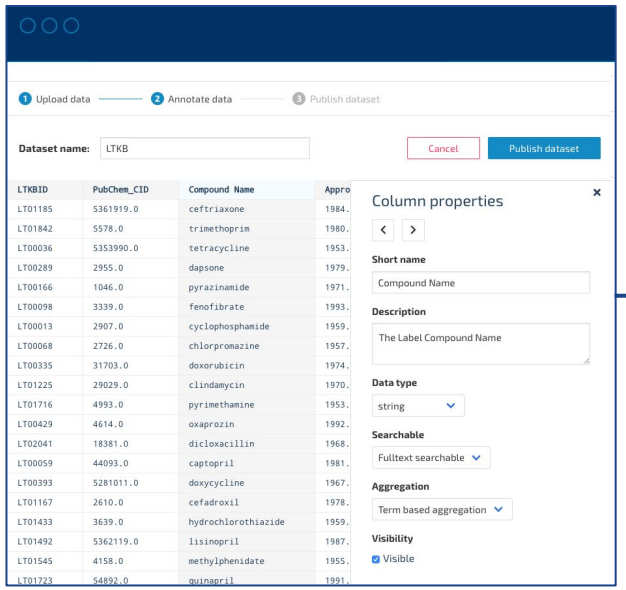

ACEnano
Knowledge Infrastructure
EdelweissData™
jupyter
CO
Laboratory
Instruments + computer & specific software
Data files
Protocols and metadata
Analysis Reporting

EdelweissData™

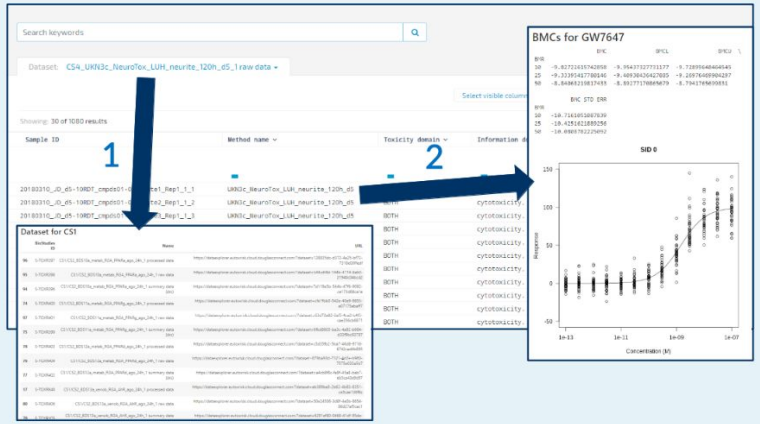
- A comprehensive tabular data and metadata environment
- Supports annotation, organisation and storage of primary data and metadata
- Provides domain data types (e.g. understand chemical's SMILES)
- Facilitates the analysis, visualisation and sharing of data
- Provides interactive exploration of the data via web-based tools
- Implements the FAIR data principles of Findability, Accessibility, Interoperability and Reusability.
- Allows the upload of data directly onto a secure, cloud-based platform
- Provides harmonised and interoperable access to different knowledge sources including publicly available databases
- Provides a rich application programming interface (API)
- Helps creating a culture of data sharing by making sharing easy
- Replace manual error-prone, time consuming and costly processes with lean data solutions and processing workflows







After indexing the data in EdelweissData, the APIs can be used to 1) show datasets from all partners relevant for a specific case study and 2) generate automatic workflows for further processing and analysis, e.g. the calculation of benchmark doses.



https://saferworldbydesign.com/edelweissdata/

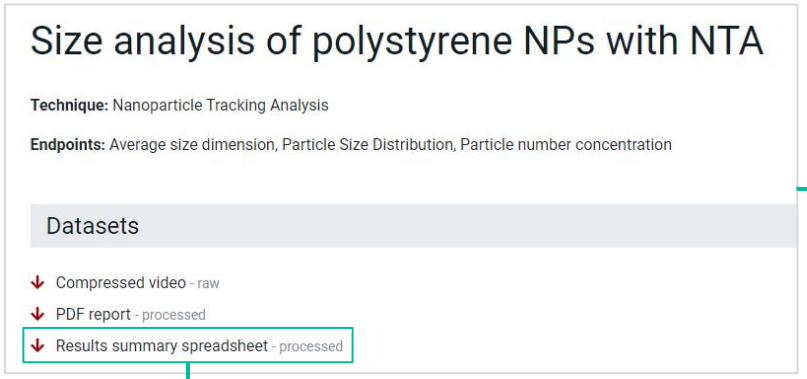
Use case: Nanoparticle Tracking Analysis (NTA)

Step 1. Addition of protocols

Step 2. Creation of data workflow

Step 3. Transfer of data to EdelweissData

- Selection of the dataset(s)
- Preparation of data file compatible with EdelweissData technology (*reading the original csv file, extracting relevant information, collecting metadata, creating the final csv summary data*)
- Automatic transfer (upload) of data
- Data visualisation



EdelweissData™

Replicate	Distribution	Weighting	Mean	Mode
1	Size	Number	97.1	97.1
2	Size	Number	95.8	95.3
3	Size	Number	96.9	97.8
4	Size	Number	96.6	96.6
5	Size	Number	95.6	95.9
1	Size	Surface Area	97.8	97.7
2	Size	Surface Area	96.4	95.8
3	Size	Surface Area	97.7	98.4
4	Size	Surface Area	97.4	97.2
5	Size	Surface Area	96.3	96.3
1	Size	Volume	98.1	97.9
2	Size	Volume	96.7	96
3	Size	Volume	98.1	98.7
4	Size	Volume	97.8	97.6
5	Size	Volume	96.5	96.5
1	Diffusion	Number	484.3	480.1
2	Diffusion	Number	492.2	489.5
3	Diffusion	Number	487.6	478.1
4	Diffusion	Number	489.9	484.7
5	Diffusion	Number	496	490.5
1	Diffusion	Surface Area	487.8	482.8
2	Diffusion	Surface Area	497.4	494
3	Diffusion	Surface Area	492.4	480.7
4	Diffusion	Surface Area	494.2	487.8
5	Diffusion	Surface Area	501.1	492.6
1	Diffusion	Volume	489.6	484.2
2	Diffusion	Volume	500.1	496.2
3	Diffusion	Volume	495.1	482.1
4	Diffusion	Volume	496.4	489.5
5	Diffusion	Volume	504.6	493.6

Step 4. Data analysis

File type: csv
Instrument: NanoSight NS300
Software: NTA 3.4 Build 3.4.003

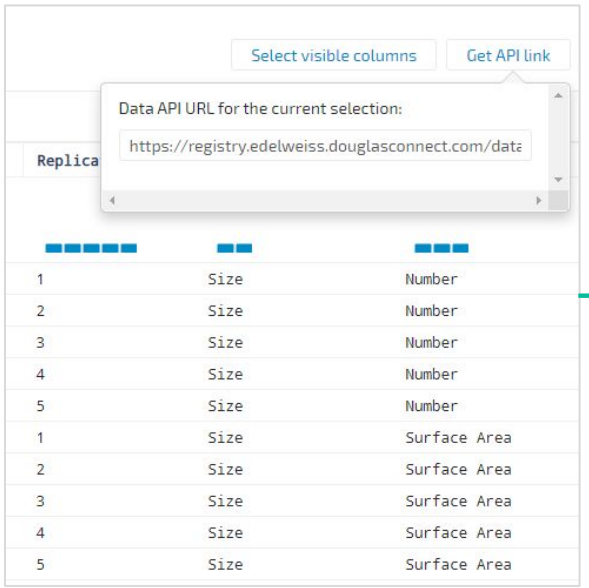
Example of summary file:
https://dataexplorer.edelweiss.douglasconnect.com/?dataset=1180f560-1eef-48d7-8fd5-f9f8bfec4446

Use case: Nanoparticle Tracking Analysis (NTA)

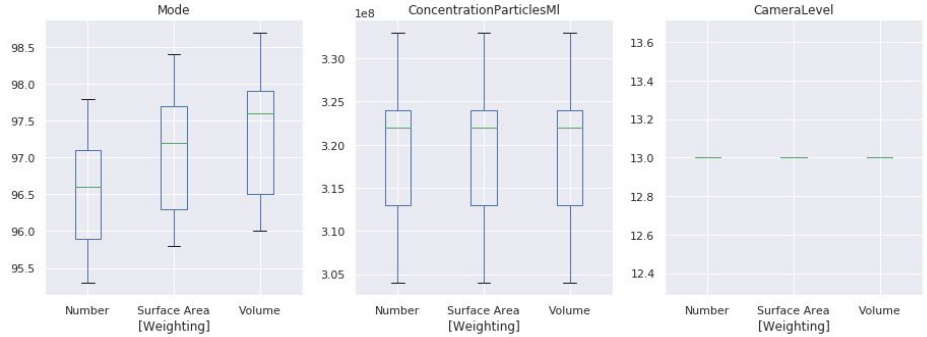
Step 4. Data analysis

- Selection of dataset(s) to be analysed: data API
- Use the data API url (e.g. in JupyterLab or Google Colaboratory tools): extraction of relevant data, analysis, plotting, etc.
- Generation of a study report

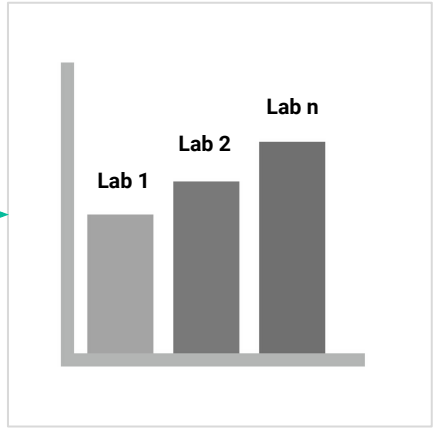
EdelweissData™



Single dataset analysis



Analysis and comparison of multiple datasets (intra- or inter-laboratory comparison studies)



Study report

Summary

Highlights

- ACEnano knowledge infrastructure (KI) supports the activities related to data collection and method optimisation in the area of physicochemical characterisation of nanomaterials.
- The KI provides a central place to access harmonised and standardised methods and data, supporting the implementation of Findable, Accessible, Interoperable and Reusable (FAIR) data principles, the reproducibility and documentation process towards the goal of generating reference resources for nanomaterials risk assessment.
- A public version of the data warehouse is being integrated in the NanoCommons data ecosystem. By semantic annotation and linking, this guarantees harmonisation and interoperability with other data sources of the EU NanoSafety Cluster.
- The protocols section facilitates access and sharing of methodology applied in nanosafety, starting with nanomaterials characterisation protocols developed or optimised within the ACEnano project.
- The experimental datasets of nanomaterials characterisation is stored together with relevant metadata pertaining to sample preparation, measurement, and the data treatment. The resulting measured value and its metadata will give as complete information as possible so that possibilities of future use of the measured value is maximised.
- The data warehouse is offering long-term storage in a re-usable format of data produced by the ACEnano project or provided by the nanosafety community.
- The development of the KI is supported by ACEnano (EU Horizon 2020 NMBP project no. 720952), while its availability to a wider community is assured by the activities in NanoCommons (Horizon 2020 INFRAIA project no. 731032).

Documentation and training materials

- User manual: https://github.com/NanoCommons/tutorials/tree/master/ACEnano manuals
- Poster summarising the KI's features: https://acenano.douglasconnect.com/dissemination/event/152/euronanoforum-2019/
- Contact and user support: acenano@edelweissconnect.com

Next training session

- Information and hands-on sessions organised during the 'EU NanoSafety Cluster Week' (10 October 2019, Copenhagen, Denmark)
- Demo session during the 'OpenTox Euro' Conference (29-31 October 2019, Basel, Switzerland)

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Analytical and Characterisation Excellence in nanomaterial risk assessment: A tiered approach

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Thank you for your attention!