



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

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NanoSafety Cluster week
10 October 2019, Copenhagen, Denmark

13:30-13:45	Welcome and overview of the program
13:45-14:30	Introduction to the Knowledge Infrastructure
14:30-15:00	Hands-on session: adding three types of protocols (sample preparation, measurement, data treatment)
15:00-15:30	<i>Coffee break</i>
15:30-17:00	Hands-on session: Creation of data workflows and upload of files Discussions on eventual issues and general user experience

The event is addressed to ACEnano project members involved in development, optimisation, validation and standardisation of methods for physico-chemical characterisation of nanomaterials.

Prerequisites and requirements for the participants:

- Each participant should have already access to the Knowledge Infrastructure;
- A laptop in order to use it independently;
- Examples of protocols used in the lab for the physico-chemical characterisation of nanomaterials (the methods applicable to ACEnano project);
- Examples of data files generated following the measurements (e.g. raw and processed files, calculations spreadsheets, etc.);

<https://tinyurl.com/y29g8pmj>
acenano@edelweissconnect.com

- Introduce the Knowledge Infrastructure (V2.0) to the project members that are involved in the experimental work
- Support project members / users in adding protocols, creating data workflows and uploading data.
- Understand more on the protocols and data annotations and the use of ontologies in the context of ACEnano.
- Discuss eventual issues related to the above topics

Following this training each participant should be familiar with the Knowledge Infrastructure and be able to add a complete data workflow, that consists of several steps:

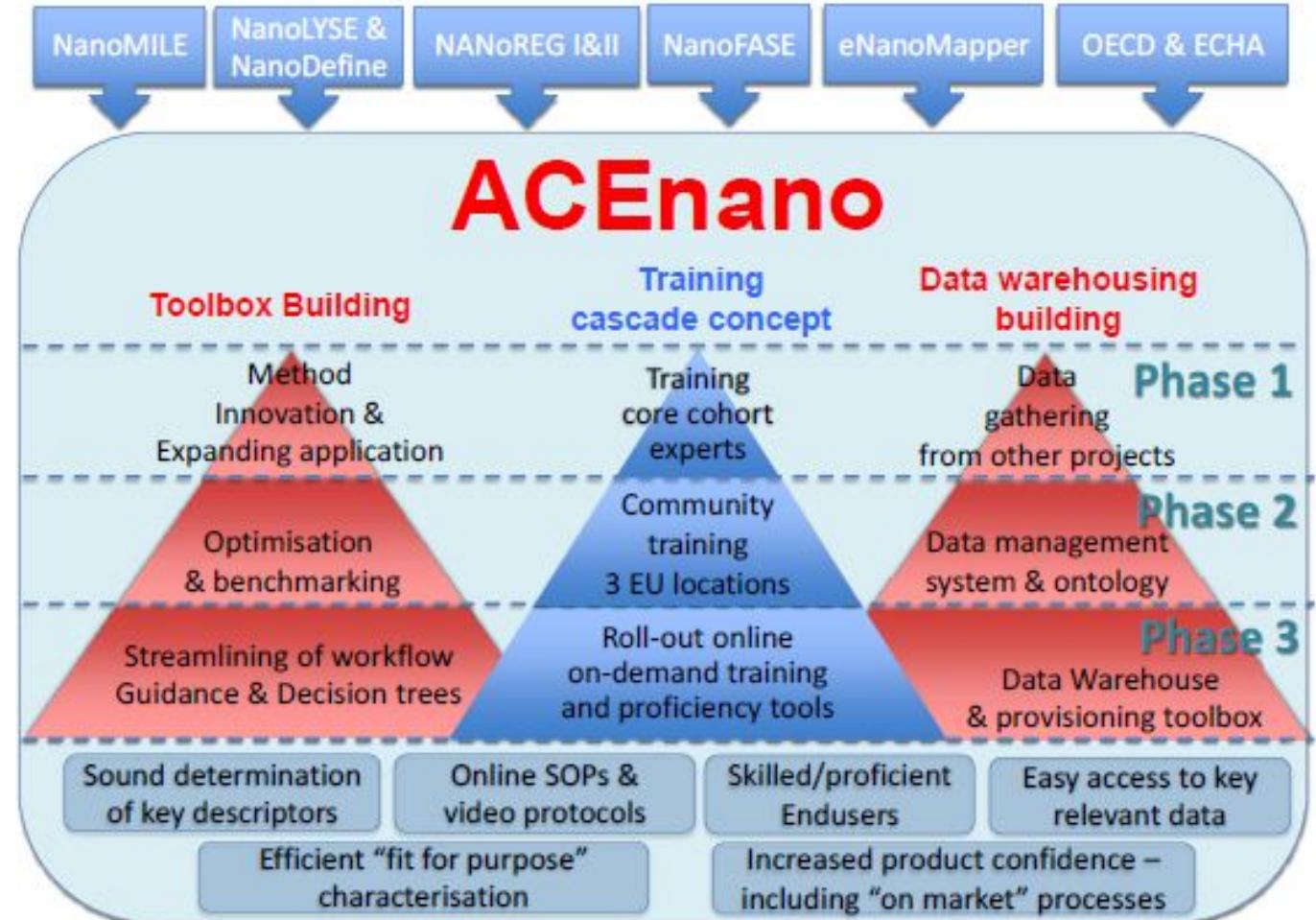
1. Add the sample preparation protocol
2. Add the measurement protocol
3. Add the data treatment protocol
4. Create the data workflow, including the description of the sample measured, and the protocols mentioned above
5. Upload raw and processed data files

Useful links and resources for participants:

- ACEnano Knowledge Infrastructure: <https://acenano.douglasconnect.com/>
- Knowledge Infrastructure Tutorial: <https://github.com/NanoCommons/tutorials/tree/master/ACEnano%20manuals>
- Article announcing **version 1.0** of the KI: <http://www.acenano-project.eu/news-events/34-release-of-acenano-knowledge-warehouse-data-collection-methods-optimisation-and-knowledge-sharing>
- Article announcing **version 2.0** of the KI: <http://www.acenano-project.eu/news-events/38-acenano-knowledge-infrastructure-version-2-0>
- Article announcing the availability of the KI to the scientific community (**public version**): <http://www.acenano-project.eu/news-events/40-acenano-knowledge-infrastructure-publicly-available-to-the-scientific-community>
- Poster: https://storage.googleapis.com/acenano/dissemination/events/2019/06/26/Poster_EuroNanoForum_2019.pdf

Introduction to ACEnano

- 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**.



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



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

Key Innovations

- Method alignment and simplification
- Comprehensive physicochemical characterisation
- Universal sample preparation and introduction systems
- Harmonisation of hardware to reduce equipment cost
- Error reduction through enhanced data management
- Method comparability enhancement

Expected impacts

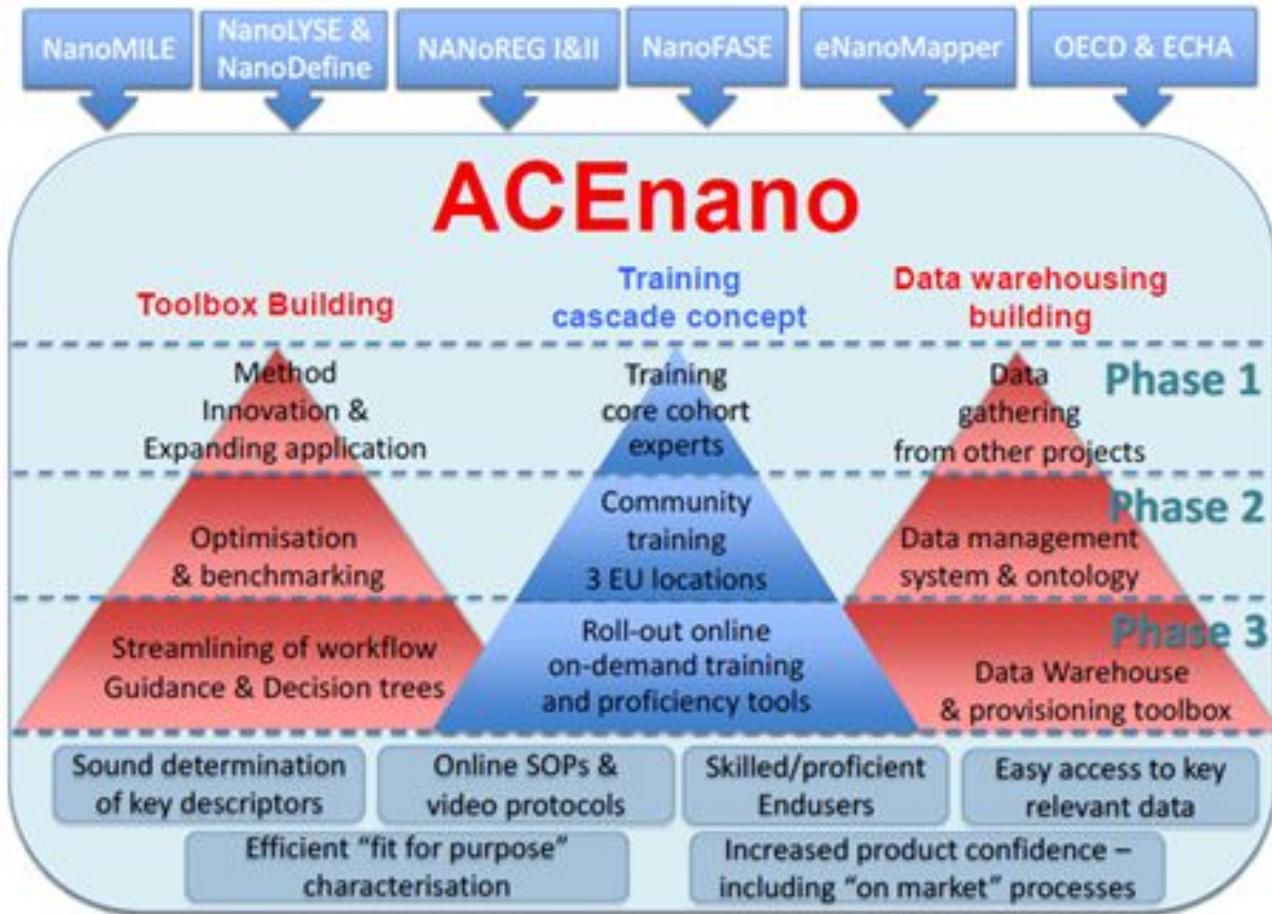
- Enable **identification of key descriptors** that reveal correlations associated with health & environmental impacts and meaningful basis for grouping, read-across and QSARs purposes
- Increase **confidence in nanosafety studies** and findings through sound physico-chemical characterisation methods and standard operating procedures
- **Reduce costs** related to the physico-chemical characterisation of nanomaterials in relevant environments
- **Identify synergies** with applications of the methods in other areas such as quality control, product traceability, labelling and counterfeiting



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

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



A tiered approach

- Method innovation on less developed techniques, optimization on existing techniques and benchmarking/standardisation of well developed techniques.
- Three layer training model:** core cohort of experts from the consortium, community training events, and other training tools.
- Data warehousing**, gathering from existing projects, defining management & ontology and provisioning the **ACENANO ToolBox**.



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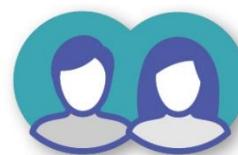
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Analytical and Characterisation Excellence in nanomaterial risk assessment: A tiered approach



Getting to efficient, cost-effective decisions on nanomaterial analysis

Iterative updating of decision schema flow based on improving knowledge of applicability domains and method accuracy and reproducibility.



Decision Tree

Integration of data into decision process including confidence levels based on previous experiments and applicability domain

Knowledge Infrastructure

Expected confidence level / applicability domain

Statistical analysis

Storing and sharing

Request for additional characterization

ACEnano methods

General quality/ reproducibility assessment of methods

Round robins

Decision Tree to guide users

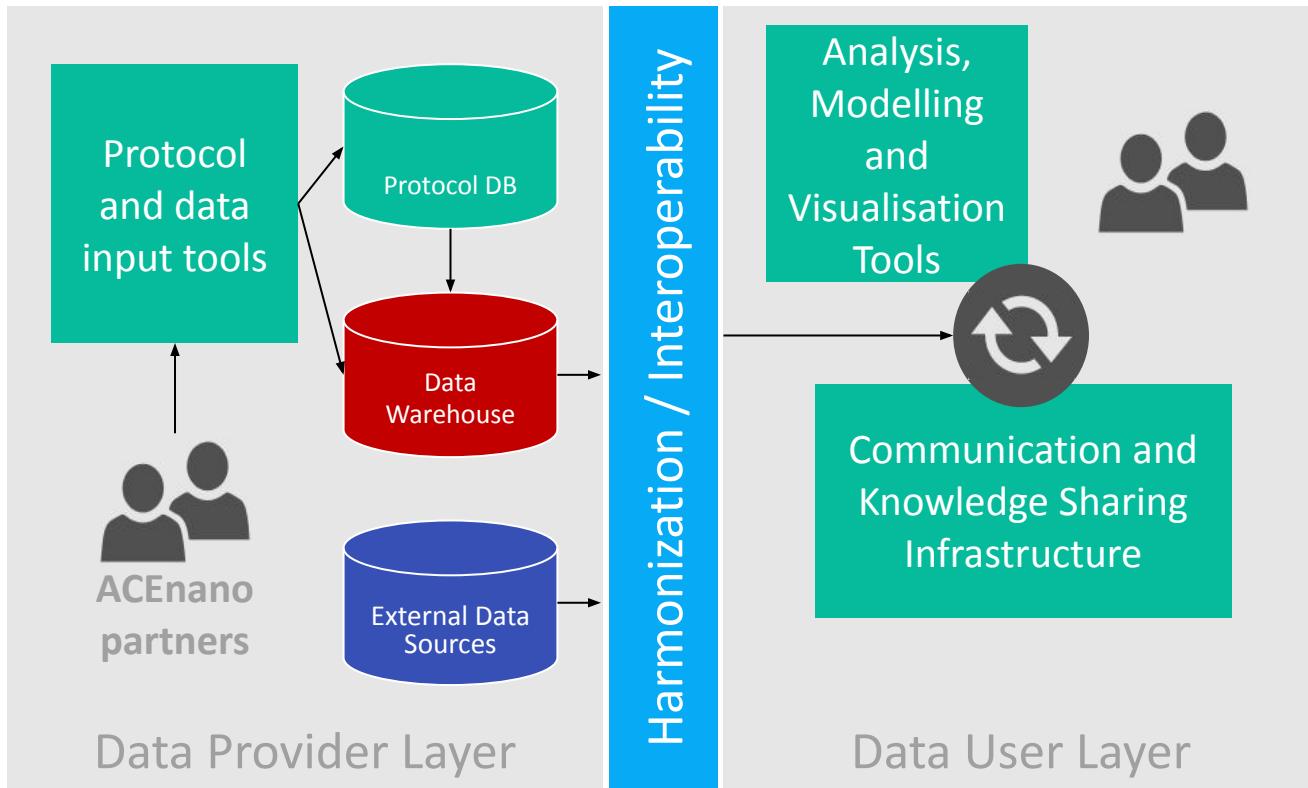
Specially for SMEs
Selection of the most appropriate methods to address their needs in risk assessment



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



→ <https://acenano.douglasconnect.com> ←

ACENANO Knowledge Warehouse

- Central place to access to nanosafety methods, including quality control guidelines and applicability domain considerations.
- Supports activities on data collection management and interpretation, ontology and methodology optimization.
- Aim to further disseminate knowledge at the level of EU NanoSafety Cluster and international NanoEHS community.
- Access to other activities and materials (e.g. dissemination activities, project library) from the project



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Introduction to the Knowledge Infrastructure

- The knowledge infrastructure (KI) supports activities related to **data collection and methodology optimisation, and aims to further disseminate this knowledge** in a re-usable format
- Supports the implementation of Findable, Accessible, Interoperable and Reusable (**FAIR**) data principles, the reproducibility of **results** and **documentation** process
- **Structured protocols** and **metadata** allow for an easier comparison of the experimental setups/protocols used and, in this way, leads to better comparability (support intra- and inter-laboratory reproducibility goal)
- Document all steps performed on a sample from the identification to the final characterisation results, solving issues on **comparability and reproducibility** of results derived from insufficient documentation of the procedures applied
- The documentation including cross-lab similarities and differences can guide the **validation and standardisation** of a method

ACEnano Knowledge Infrastructure
<https://aceno.douglasconnect.com/>

A central platform to access harmonised and standardised methods applied for physicochemical characterisation of nanomaterials

Protocols

Compilation of protocols (methods) used or developed in the project.

[View the protocols >](#)

Data

Collection of ACEnano data and experimental results.

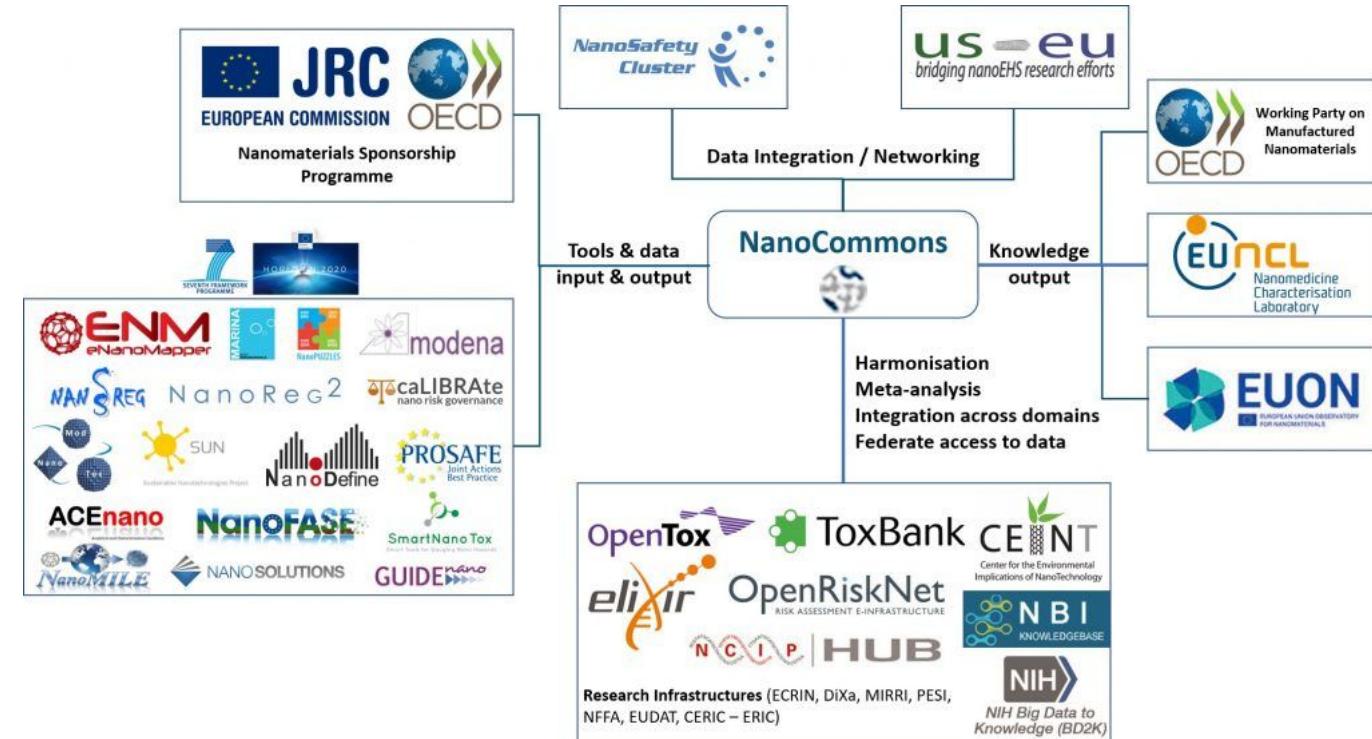
[Explore the data >](#)

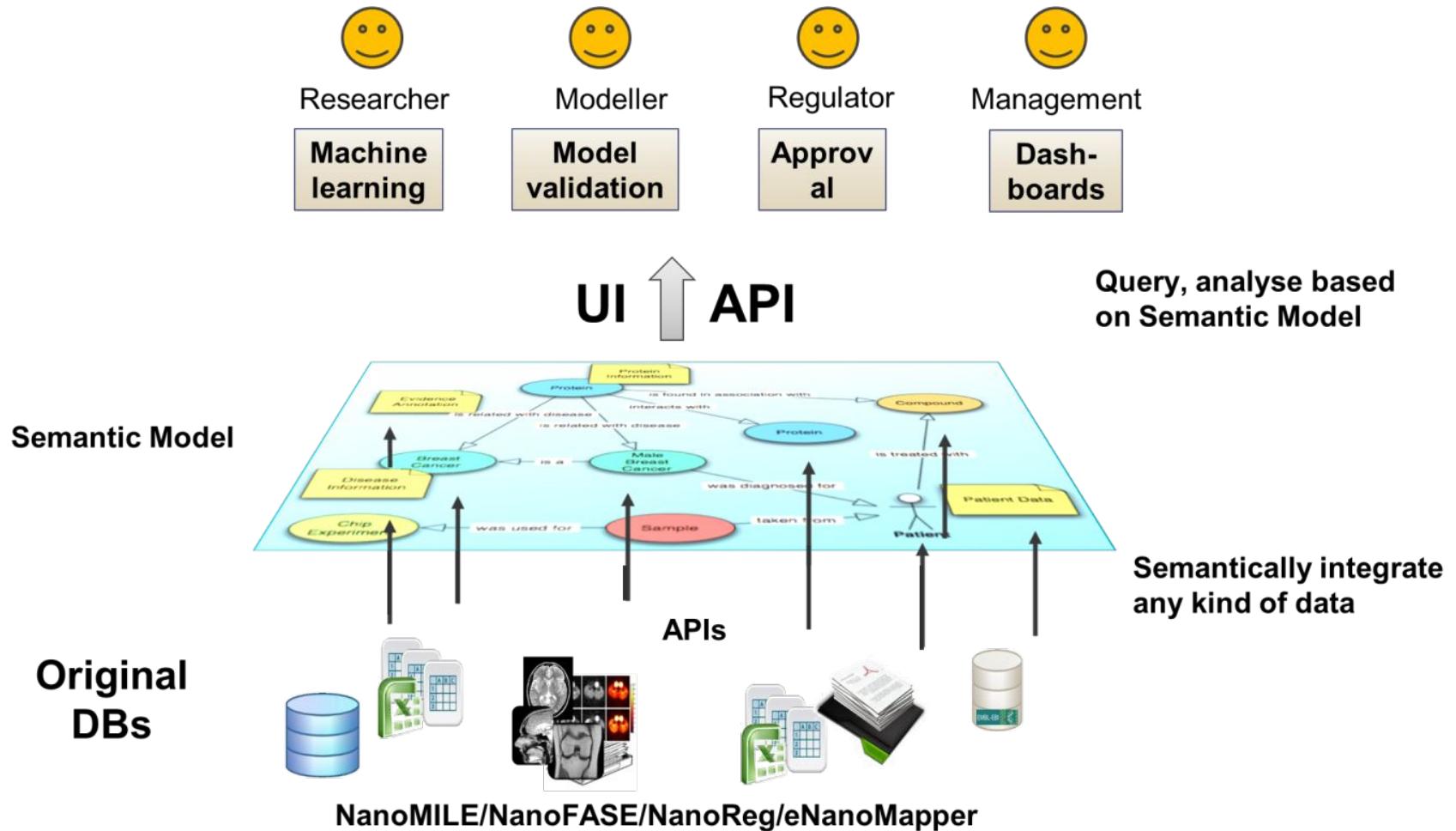
Dissemination

Collection of dissemination publications and events related to the ACEnano project.

[Dissemination activities >](#)

- **NanoCommons** (Horizon 2020; Project number 731032) will deliver a sustainable and openly accessible nanoinformatics framework (knowledgebase and integrated computational tools, supported by expert advice, data interpretation and training), for assessment of the risks of NMs, their products and their formulations.





Public version provided
and integrated by



NanoCommons
Nano-Knowledge Community

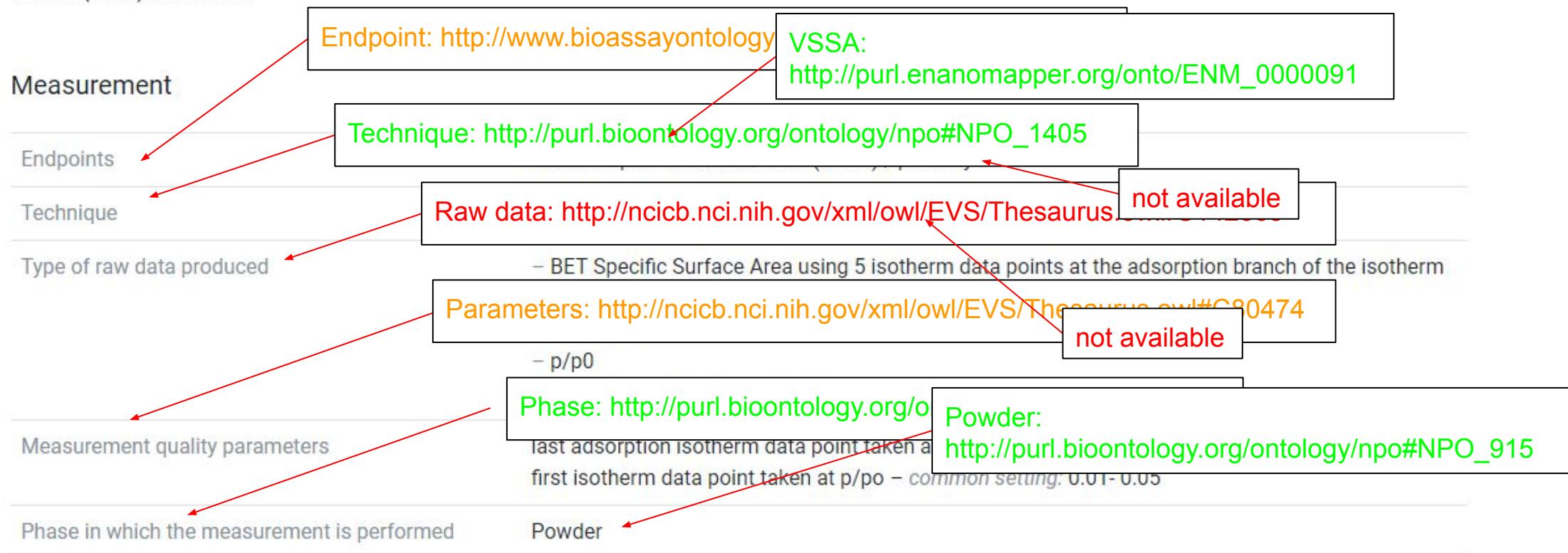


This project has received funding from the European Union Horizon 2020
Programme (H2020) under grant agreement no. 731032

Sample Analysis BET UoB test

Measurement protocol

This protocol describes the measuring of the amount of physically adsorbed gas according to the Brunauer, Emmett and Teller (BET) method.



Instrument

Instrument: http://purl.bioontology.org/ontology/npo#NPO_1436

Instrument

Parameters: <http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C80474>

Settings and parameters

not available

Setting	Value	Unit
N2	1.5	bar
He (or other inert gas in use)	2.0	bar
Warming time	20	min

Upper limit of detection

200 mg

Lowest limit of detection

100 mg

Lowest limit of detection:
<http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C80474>

Steps

Warming time: not available
Time: http://www.ebi.ac.uk/efo/EFO_0000721
Minute: http://purl.obolibrary.org/obo/GO_0000031

- 1 Switch on the BET instrument and wait 20 minutes for it to warm up.

If needed, switch on the vacuum pump.

Description of Sample

Nanoparticles in sample

Name:	CAS number:
titanium dioxide nano	
titanium dioxide nanoparticle response pathway http://purl.obolibrary.org/obo/PW_0001437 A pathway triggered by exposure to titanium dioxide nanoparticle (nano-TiO ₂). Nano-TiO ₂ has a broad range of applications but studies indicate that under conditions of long and high dose exposure, it can exert cytotoxic and genotoxic effects. Nano-TiO ₂ has been shown to induce inflammation, oxidative stress and MAP kinase activity.	
titanium dioxide nanoparticles http://purl.obolibrary.org/obo/XCO_0000339 Any condition in which the main	
Crystalline phase:	
Size units:	<input type="text" value="nano"/> nano http://purl.obolibrary.org/obo/UO_0000300 A prefix in the metric system denoting a factor of 10 to the power of -9.
	nanoliter http://purl.obolibrary.org/obo/UO_0000102 A volume unit which is equal to one thousandth of one millionth of a liter or 10 ⁻⁹ L.
	nanometer http://purl.obolibrary.org/obo/UO_0000018 A length unit which is equal to one thousandth of one millionth of a meter or 10 ⁻⁹ m.

Addition of media or compounds during sample preparation

Add a new medium

Name:	PBS
PbSub2 http://purl.obolibrary.org/obo/IDOMAL_0001082 A secreted protein expressed in ookinete stage forming protein aggregates that are often associated with the actin cytoskeleton.	
PBS buffer http://purl.obolibrary.org/obo/MSIO_0000021 Phosphated buffer saline (PBS) buffer is a buffer which is a water-based salt solution containing disodium hydrogen phosphate, sodium chloride and, in some formulations, potassium chloride and potassium dihydrogen phosphate.	

Compound name:	sodium ch
sodium chloride http://purl.obolibrary.org/obo/CHEBI_65242 An inorganic sodium salt that has chlorate as the counter-ion. An oxidising agent, it is used for bleaching paper and as a herbicide. It is also used in the manufacture of dyes, explosives and matches.	
sodium chlorite http://purl.obolibrary.org/obo/CHEBI_78667 An inorganic sodium salt in which chlorite is the counterion.	
sodium chloride http://purl.obolibrary.org/obo/CHEBI_26710 An inorganic chloride salt having	

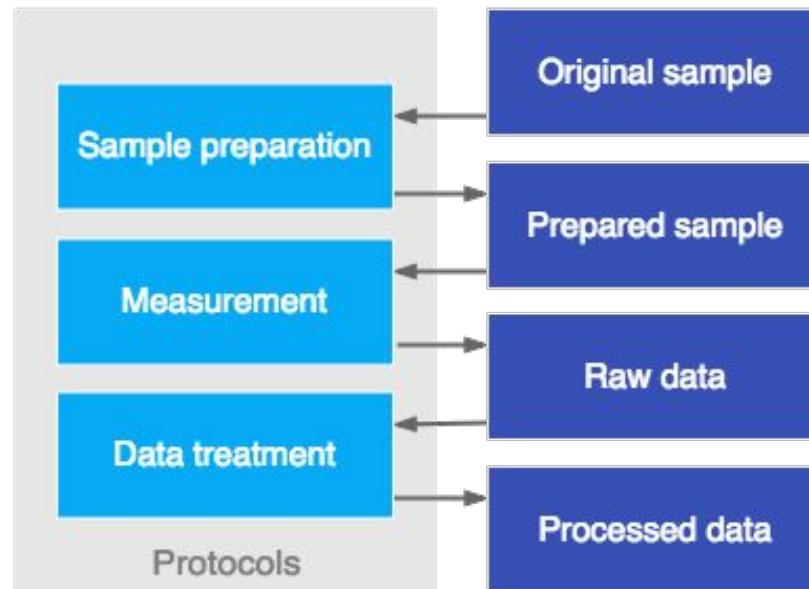
Collection of required new classes

Warehouse Term	Ontology URL	BioPortal Description	Comparation Descriptions	Specialists Description
Wide-Angle X-ray Scattering	http://purl.obolibrary.org/obo/CHMO_0000207	A method for determining structure by measuring the change in direction or energy of X-rays scattered by a sample at wide angles (>10 deg.). Wide-angle X-ray scattering is used for determining the structure of polymers.	Missing Specialist	NA
Conductivity	http://purl.obolibrary.org/obo/NCIT_C134263	A measure of the ion-facilitated electron current through a material.	Missing Specialist	NA
Extractant	NA	NA	Missing Specialist	NA
Ionic strength	http://purl.obolibrary.org/obo/NCIT_C52478	The weighted concentration of ions in solutions.	Missing Specialist	NA
Purity (resistivity)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C62352	A quantitative assessment of the homogeneity or uniformity of a mixture. Alternatively, purity refers to the degree of being free of contaminants or heterogeneous components.	Missing Specialist	NA
Viscosity	http://purl.obolibrary.org/obo/NCIT_C75912	The resistance of a liquid to sheer forces and flow.	Missing Specialist	NA
Limit of Quantification- must be added in KI! Or add "Lower limit of detection" to eNM?	http://purl.obolibrary.org/obo/CHMO_0002802	The smallest measure that can be quantified with reasonable certainty for a given analytical procedure.	Missing in KI	Limit of quantification is the value which gives you the lowest, reliable quantifiable amount of a compound
Upper limit of detection	NA	NA	Missing in BioPortal	The largest value measurable using a defined method
Density	http://purl.enanomapper.org/onto/ENM_0000084	ENM	Missing in BioPortal	Mass per unit of volume
Dilution scale factor	NA	NA	Missing in BioPortal	The degree to which the concentration of a analyte has been reduced. 2. We only use dilution factor
Drying	http://purl.bioontology.org/ontology/npo#NPO_1956	ENM	Missing in BioPortal	The removal of water or solvent from a sample by evaporation
Vortexing	http://purl.bioontology.org/ontology/npo#NPO_1952	ENM	Missing in BioPortal	The mixing of liquids to produce a more homogenous sample using cyclic motion to produce a vortex
Dilution	???	NA	Missing in BioPortal	Reduction in concentration of an analyte
Sonication	http://purl.bioontology.org/ontology/npo#NPO_1961	ENM	Missing in BioPortal	The use of sound energy typically ultra hgh frequency to agi or mix samples
Heating	http://purl.bioontology.org/ontology/npo#NPO_1958	ENM	Missing in BioPortal	Increasing temperature
Milling	???	NA	Missing in BioPortal	The use of rotational cutting or grinding to reduce the size o bulk material

https://docs.google.com/spreadsheets/d/1mqt4epvvXMDFjpO5KeY_2u135WFXAhJfEXY4mkZH-A/edit

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

Endpoint	Techniques
Average size dimension	DLS - Dynamic Light Scattering Mastersizer - Mastersizer NTA - Nanoparticle Tracking Analysis SAXS - Small-Angle X-ray Scattering TEM - Transmission Electron Microscopy UV-Vis - Ultraviolet-visible spectroscopy WAXD - Wide-Angle X-ray Scattering XRD - crystallite size - X-Ray Diffraction - crystallite size
Batch dispersion / stability	DLS - Dynamic Light Scattering
Corona characterisation	CE-MS - Capillary electrophoresis-Mass Spectrometry
Crystalline phase	TEM - Transmission Electron Microscopy XRD - crystalline phase - X-Ray Diffraction - crystalline phase
Density	cF3 - Centrifugal field flow fractionation Disc centrifuge - Disc centrifuge
Deposition rate	Column test - Column test QCMD - Quartz crystal microbalance with dissipation monitoring
Elemental composition and chemical purity	SEM/TEM-EDX - Energy Dispersive X-ray Spectroscopy in the SEM and TEM ICP-MS - Inductively Coupled Plasma Mass Spectrometry LA-ICP-MS - Laser Ablation Inductively Coupled Plasma Mass Spectrometry LDI-TOF-MS - Laser Desorption/Ionization Time of Flight Mass Spectrometry MALDI-TOF-MS - Matrix-Assisted Laser Desorption/Ionization Time of Flight Mass Spectrometry SP-TOF-ICP-MS - Single Particle Time of flight Inductively Coupled Plasma Mass Spectrometry TOF-SIMS - Time of flight secondary ion mass spectrometry

Functional coating

CE - Capillary electrophoresis
LDI-TOF-MS - Laser Desorption/Ionization Time of Flight Mass Spectrometry
MALDI-TOF-MS - Matrix-Assisted Laser Desorption/Ionization Time of Flight Mass Spectrometry
QCMD - Quartz crystal microbalance with dissipation monitoring
Raman - Raman spectroscopy
STEM-EDS - Scanning Transmission Electron Microscope- Energy-dispersive X-ray spectroscopy
TGA-IR-GC/MS - Thermogravimetric analysis coupled with IR-GC or MS
TOF-SIMS - Time of flight secondary ion mass spectrometry
TERS - Tip Enhanced Raman Scattering (nano-Raman)
XPS - X-Ray photon spectroscopy

Homoaggregation rate

CE - Capillary electrophoresis
Time resolved DLS - Time resolved Dynamic Light Scattering
Time resolved SP-ICP-MS - Time resolved Single Particle Inductively Coupled Plasma Mass Spectrometry
Time resolved NTA - Time resolved nanoparticle tracking analysis

Hydrophobicity

Assay-on-a-chip - Assay-on-a-chip
Dye loaded FFF - Dye loaded field flow fractionation
Force tensiometry - Force tensiometry
HIC - Hydrophobic interaction chromatography

Isoelectric Point

EM - Electrophoretic mobility

NP-cell interaction

Assay-on-a-chip - Assay-on-a-chip
QCMD - Quartz crystal microbalance with dissipation monitoring

Particle Size Distribution

aF4 - Asymmetrical field flow fractionation
AFM - Atomic Force Microscopy
CE - Capillary electrophoresis
cF3 - Centrifugal field flow fractionation
Disc centrifuge - Disc centrifuge
Mastersizer - Mastersizer
NTA - Nanoparticle Tracking Analysis
SEC/HDC/HIC - SEC/HDC/HIC
SEM - Scanning Electron Microscopy
SP-ICP-MS - Single Particle Inductively Coupled Plasma Mass Spectrometry
SC-spICP-MS - Single-cell Single Particle Inductively Coupled Plasma Mass Spectrometry
TEM - Transmission Electron Microscopy
UV-Vis - Ultraviolet-visible spectroscopy

Particle number concentration

LIBD - Laser induced breakdown detection
 NTA - Nanoparticle Tracking Analysis
 SEM - Scanning Electron Microscopy
 SP-ICP-MS - Single Particle Inductively Coupled Plasma Mass Spectrometry
 TEM - Transmission Electron Microscopy



Particle shape

AFM - Atomic Force Microscopy
 Centrifugal FFF-MALS - Centrifugal Field-Flow Fractionation-MALS
 MALS/SLS - MALS/SLS
 SEM - Scanning Electron Microscopy
 SAXS - Small-Angle X-ray Scattering
 TEM - Transmission Electron Microscopy

ROS generation

Redox speciation

TXM - Full field transmission X-ray microscopy
 STXM - Scanning transmission X-ray microscopy
 TEM-EELS - Transmission electron microscopy with electron energy loss spectroscopy
 XPS - X-Ray photon spectroscopy
 XANES - X-ray absorption near edge spectroscopy

Solubility/dissolution

Assay-on-a-chip - Assay-on-a-chip
 Dialysis + ICP-MS - Dialysis + ICP-MS
 Ion-selective electrode - Ion-selective electrode
 NTA - Nanoparticle Tracking Analysis
 SP-ICP-MS - Single Particle Inductively Coupled Plasma Mass Spectrometry
 Ultracentrifugation + ICP-MS - Ultracentrifugation + ICP-MS
 Ultrafiltration + ICP-MS - Ultrafiltration + ICP-MS

Volume Specific Surface Area (VSSA) / porosity

BET - Brunauer–Emmett–Teller analysis
 NMR relaxation - Nuclear magnetic resonance spectroscopy relaxation

Z-potential

ELS - Electrophoretic Light Scattering
 EM - Electrophoretic mobility

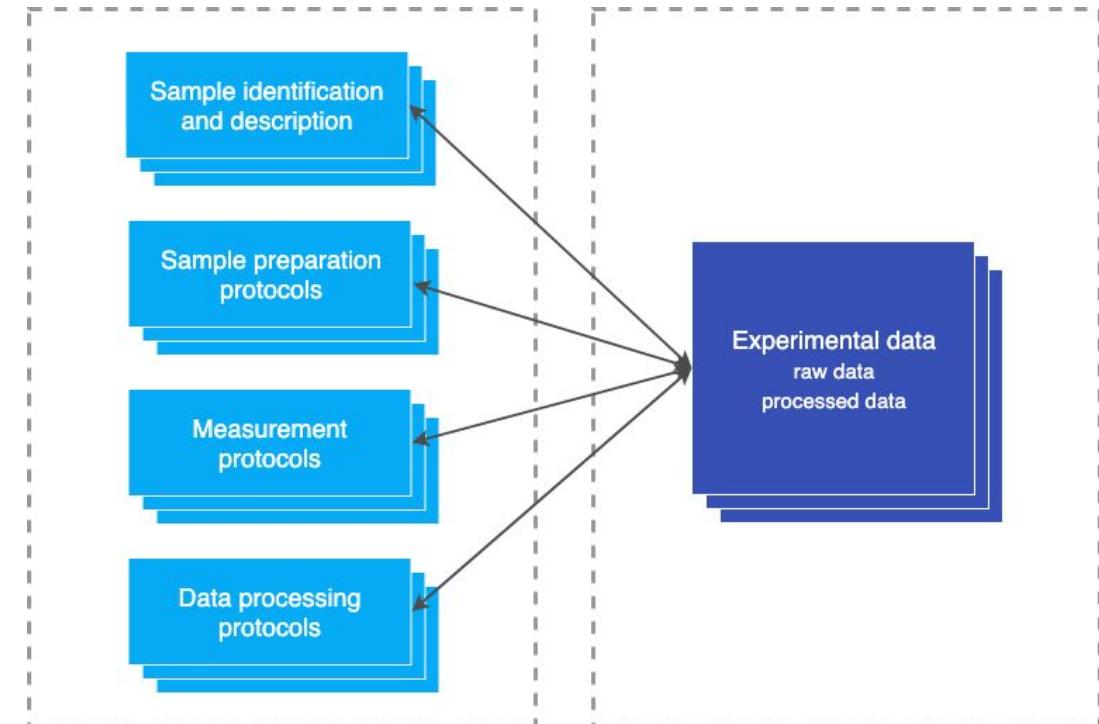
Sample preparation protocol	
Part 1: General information	Protocol name and description
	Contacts
	Technique and Endpoints
Part 2: Steps	Multiple actions and action parameters
→ Preview protocol, Make more changes & Submit protocol	

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	

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	

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.





7

Data files

Dataset type: Raw	Dataset name: <input type="text"/>	Upload dataset: <input type="button" value="Choose File"/> No file chosen
<input type="checkbox"/> Delete this dataset		
Dataset type: Processed	Dataset name: <input type="text"/>	Upload dataset: <input type="button" value="Choose File"/> No file chosen
<input type="checkbox"/> Delete this dataset		
+ Add dataset		
Submit your data		

Analysis

Technique	Organisation	Filter	Reset
Characterisation of gold nanoparticles			
Technique: Ultraviolet-visible spectroscopy			
Endpoint: Average size dimension			
ACEnano_UVVis_Raw data_AuNP 20190605			
Raw			5 Jun 2019
ACEnano_UVVis_Results_AuNP 20190605			
Processed			
Particle Size Distribution by UV-Vis 20190603			
Technique: Ultraviolet-visible spectroscopy			
Endpoint: Particle Size Distribution			
Particle size distribution test 20190603			
Raw			3 Jun 2019
Particle size distribution test 20190603			
Raw			

View complete workflow

Characterisation of gold nanoparticles

This workflow describes the sample preparation, measurement and data treatment procedures for particle size measurements of gold NP suspensions. The procedure involves quantification of the extinction of light that is measured from the spectral pattern using absorbance. UV-Vis refers to the ultraviolet to visible spectral region of light, the absorption of which is size dependent at the nanoscale. UV-Vis is therefore an ideal technique for the size characterisation of NP suspensions through absorbance at an appropriate wavelength. The settings defined below will be refined to optimise results during the subsequent runs.

Technique: Ultraviolet-visible spectroscopy
Endpoints: Average size dimension

Datasets

- ACEnano_UVVis_Raw data_AuNP 20190605 - raw
- ACEnano_UVVis_Results_AuNP 20190605 - processed

Sample description

Name: Gold nanoparticles
Code: AuNP BBI Unknown
Supplier: BBI Solutions OEM Ltd
Medium: Unknown
Phase: Aqueous liquid
Sample volume: 1 mL
Concentration of material in sample: 50 mg/L

Nanoparticle

Core chemistry: Au
CAS number: 7440-57-5
Size: Unknown nm

Sample preparation protocol

For technique: Ultraviolet-visible spectroscopy
For endpoints: Average size dimension, Particle Size Distribution

- Vortexing** Mixing and dispersing of nanoparticles that are suspended in a liquid phase
Speed: /
Duration: 2 min
Phase change: Aqueous liquid → Aqueous liquid
- Dilution** Additional dilution of original sample for analysis

Data - view, filter, analyse, API

EdelweissData™ Explorer

Showing: 6 of 6 rows

Technique	Endpoint	Endpoint measure	Phase in which the measure...	Instrument	Type of instrument	Software version
Ultraviolet-visible spectrophot...	Particle size distribution	Absorption	Aqueous liquid	UVVis Spectrometer	Jenway 6800	Flight Deck - 1.0
Ultraviolet-visible spectrophot...	Particle size distribution	Absorption	Aqueous liquid	UVVis Spectrometer	Jenway 6800	Flight Deck - 1.0
Ultraviolet-visible spectrophot...	Particle size distribution	Absorption	Aqueous liquid	UVVis Spectrometer	Jenway 6800	Flight Deck - 1.0
Ultraviolet-visible spectrophot...	Particle size distribution	Absorption	Aqueous liquid	UVVis Spectrometer	Jenway 6800	Flight Deck - 1.0
Ultraviolet-visible spectrophot...	Particle size distribution	Absorption	Aqueous liquid	UVVis Spectrometer	Jenway 6800	Flight Deck - 1.0
Ultraviolet-visible spectrophot...	Particle size distribution	Absorption	Aqueous liquid	UVVis Spectrometer	Jenway 6800	Flight Deck - 1.0

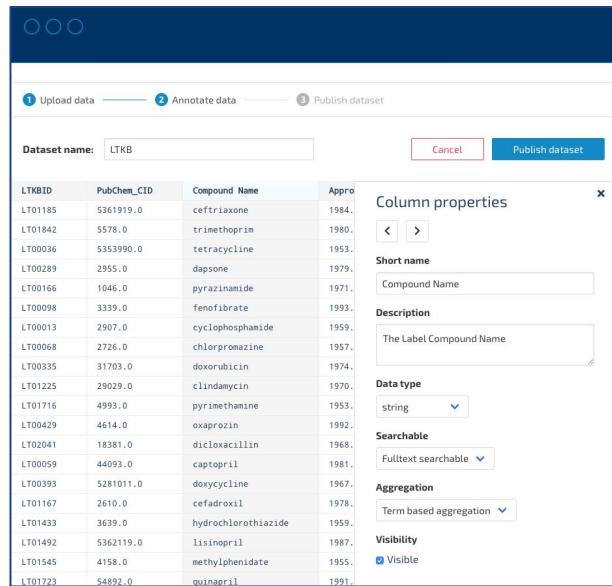
Showing: 6 of 6 rows

Start Wavelength	End Wavelength	Sample name	Sample code	Supplier	Phase	Core chemistry
680 nm	380 nm	Gold nanoparticles	AuNP 5 nm	BBI Solutions OEM Ltd	Aqueous liquid	Au
680 nm	380 nm	Gold nanoparticles	AuNP 20 nm	BBI Solutions OEM Ltd	Aqueous liquid	Au
680 nm	380 nm	Gold nanoparticles	AuNP 40 nm	BBI Solutions OEM Ltd	Aqueous liquid	Au
680 nm	380 nm	Gold nanoparticles	AuNP 60 nm	BBI Solutions OEM Ltd	Aqueous liquid	Au
680 nm	380 nm	Gold nanoparticles	AuNP 100 nm	BBI Solutions OEM Ltd	Aqueous liquid	Au
680 nm	380 nm	Gold nanoparticles	AuNP BBI Unknown	BBI Solutions OEM Ltd	Aqueous liquid	Au

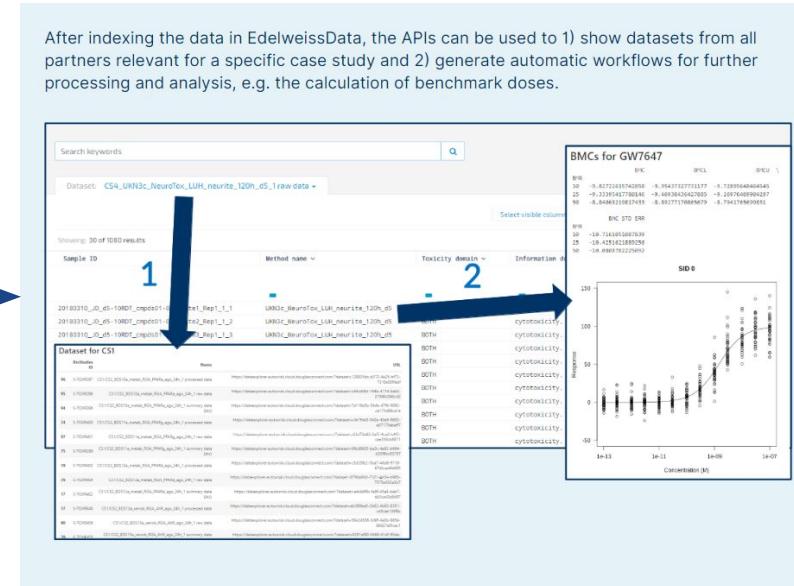
EdelweissData™

Size	Size unit	Stock concentration	Stock concentration unit	Max absorption wavelength	Absorbance	Measured size
5	nm	50	mg/L	547	0.402	
20	nm	50	mg/L	524	0.501	
40	nm	50	mg/L	530	0.547	
60	nm	50	mg/L	534	0.666	
100	nm	50	mg/L	571	0.47	
Unknown	nm	50	mg/L	548	0.719	78

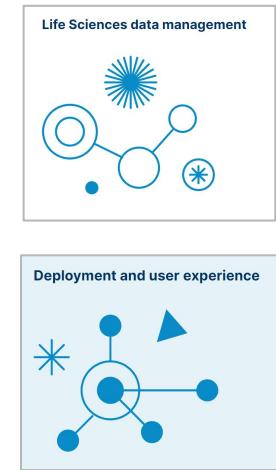
- A comprehensive tabular data and metadata environment
- Supports annotation, organisation and storage of primary data and metadata
- Provides domain data types (e.g. understand chemical's SMILES)
- Facilitates the analysis, visualisation and sharing of data
- Provides interactive exploration of the 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

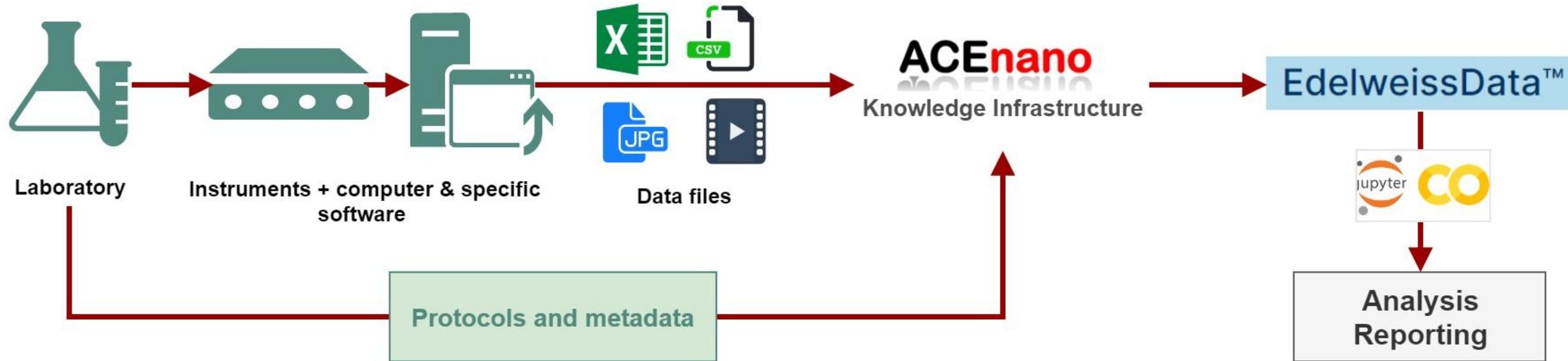


The screenshot shows the EdelweissData interface for managing datasets. At the top, there are tabs for 'Upload data', 'Annotate data', and 'Publish dataset'. Below this, a search bar contains 'LTKB'. A table lists various compounds with their IDs, PubChem_CIDs, names, and approval years. To the right of the table is a 'Column properties' modal window. This modal includes fields for 'Short name' (set to 'Compound Name'), 'Description' ('The Label Compound Name'), 'Data type' ('string'), 'Searchable' ('Fulltext searchable'), 'Aggregation' ('Term based aggregation'), and 'Visibility' ('Visible').



The screenshot shows the EdelweissData search and analysis interface. On the left, a search results page displays 30 of 1080 results for the dataset 'CS4_UNINc_NeuroTox_UH_neurite_120h_d5_1.raw data'. The results are listed in a table with columns for 'Sample ID', 'Method name', 'Toxicity domain', and 'Information'. An arrow labeled '1' points from the search results to a detailed view of a specific dataset entry. Another arrow labeled '2' points from the detailed view to a toxicity plot titled 'BMCS for GW7647'. The plot shows cytotoxicity data with 'SID 0' on the y-axis and 'Concentration (M)' on the x-axis, featuring a logarithmic scale.





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

Size analysis of polystyrene NPs with NTA

Technique: Nanoparticle Tracking Analysis

Endpoints: Average size dimension, Particle Size Distribution, Particle number concentration

Datasets

- Compressed video - raw
- PDF report - processed
- Results summary spreadsheet - processed

EdelweissData™

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

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	479.1
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

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

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™

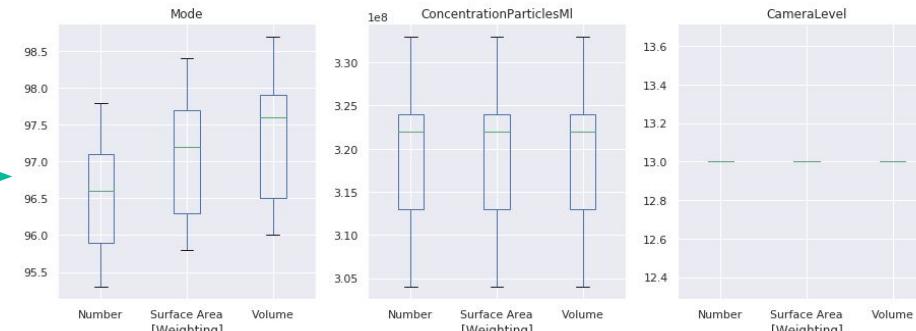
Select visible columns Get API link

Data API URL for the current selection:
<https://registry.edelweiss.douglasconnect.com/data>

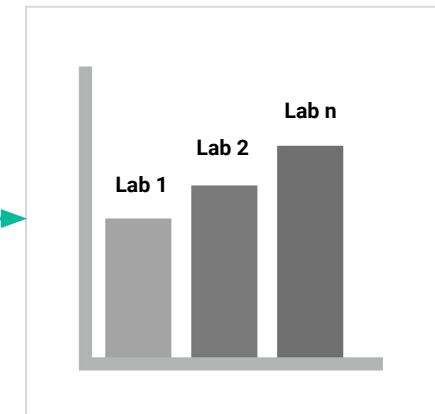
Replica	Size	Number
1	Size	Number
2	Size	Number
3	Size	Number
4	Size	Number
5	Size	Number
1	Size	Surface Area
2	Size	Surface Area
3	Size	Surface Area
4	Size	Surface Area
5	Size	Surface Area



Single dataset analysis



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



Study report

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).

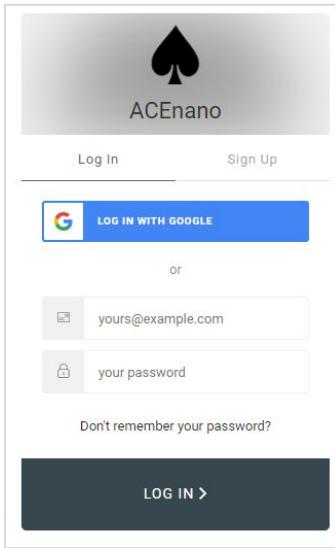
Documentation and training materials

- User manual: <https://github.com/NanoCommons/tutorials/tree/master/ACEnano%20manuals>
- 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

- Demo session during the 'OpenTox Euro' Conference (29-31 October 2019, Basel, Switzerland)

Access to the platform, establish the cases (techniques and endpoints) covered, splitting of participants in groups



ACEnano Knowledge Infrastructure

This platform is the Knowledge Infrastructure of the ACEnano Project - Analytical and Characterisation Excellence in nanomaterial risk assessment: a tiered approach. ACEnano aim to introduce confidence, adaptability and clarity into nanomaterial risk assessment by developing a widely implementable and robust tiered approach to nanomaterials physicochemical characterisation that will simplify and facilitate contextual (hazard or exposure) description and its transcription into a reliable nanomaterials grouping framework.

[About ACEnano >](#)

LATEST POSTS - DATA AND PROTOCOLS

Data	Size determination of gold nanoparticles by Asymmetrical Flow Field-Flow Fractionation	5 Sep 2019
The purpose of this data protocol is to provide guidelines for sample preparation and size determination of gold nanoparticles in suspension in the size range between 20 and 100 nm using AF4. Sample preparation, fractionation and data analysis need to be standardised and well-documented in order to enable comparable, repeatable and reproducible results throughout all participating laboratories. Analysis workflow		
Protocol	Evaluation AuNP Round Robin FFF	5 Sep 2019
Data treatment protocol		
Protocol	AuNP round robin FFF	4 Sep 2019
Size determination of gold nanoparticles by Asymmetrical Flow Field-Flow Fractionation coupled with UV-vis-detection Measurement protocol		
Protocol	Sample preparation protocol AuNP round robin FFF	4 Sep 2019
Sample preparation protocol		
Data	NTA round robin AuNP	5 Jul 2019
Au particles ~ 60 nm diameter Analysis workflow		

EXPLORE

Protocols
Compilation of protocols (methods) used or developed in the project.
[View the protocols >](#)

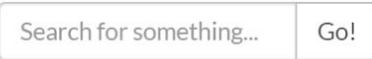
Data
Collection of ACEnano data and experimental results.
[Explore the data >](#)

Dissemination
Collection of dissemination publications and events related to the ACEnano project.
[Dissemination activities >](#)

User manual:

<https://github.com/NanoCommons/tutorials/tree/master/ACE nano manuals>

- How to access the knowledge infrastructure
- The main features of the knowledge infrastructure
- How to add a new protocol
- How to create a new data workflow
- How to request support or suggest improvements of the platform



Hi, Thomas Exner



UoB UV-Vis Round Robin

PROTOCOLS

RESULTS

ACTIVITY

INVENTORIES ▾

ARCHIVED RESULTS

1 1. Materials and Methods | Published on 07/13/2018 12:51 by NanoCommons

Complete Step

**1.1 Essential equipment**

1. UV-Vis Spectrophotometer.
2. Calibrated Volume Pipettors of 1 and 5 mL with disposable tips.
3. Disposable 3mL cuvettes (Suggested: polystyrene 10 x 10 x 45mm, SARSTEDT, Catalogue number: 67.742).

1.2 Chemicals

1. Ultrapure water 18.2 MΩcm.

1.3 Materials supplied

Monodisperse BBI AuNP stock suspensions (1 mL, MSDS attached) in sizes of 5, 20, 40, 60, and 100 nm. The concentration of all stock suspensions is 50 mg/L. A monodispersed BBI AuNP suspension having an unknown size (1 mL). The received samples should have a red tinge (Figure 1) and be stored at 4-8°C. Kindly contact UoB (details below) if you believe that the samples have been compromised during shipping. It should be aimed that samples are analysed as shortly after arrival as possible.



<https://tinyurl.com/y29g8pmj>

1. ACEnano_DataManagementTraining_NSCweek20191010.pdf
2. ACEnano Data Management Training 10 Oct 2019
3. ACEnano Knowledge Warehouse 09 Oct 2019
4. UV-Vis-Protocol.pdf - protocol exported from SciNote
5. RawData.xlsx
6. UV-VIS_data_.xlsx - data from round robin

Hands-on session: 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	

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	

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	

Part 1: General information

Protocol name and description

Protocol names

Protocols may have two identifiers/names:

1. **Original name:** this is the original/published name of the protocol or tradename. It is not mandatory.
2. **ACEnano ID:** this will be the assigned name of the protocol for the ACEnano data base. The name is assembled from the acronym of the organisation that is submitting the protocol, from the type of protocol and from the protocol version and variant, if provided (e.g. ACEnano_DC_DLS_1_a).

Organisation submitting the protocol:

EwC - Edelweiss Connect GmbH

Protocol original name:

Original/published name or tradename.

Version of this protocol:

Variant of this protocol:

Use numbers to identify the versions of the protocol (e.g. 1, 2, ...). A new version is an updated version of the same protocol (e.g. major changes in the protocol steps, change of the instruments used for measurements, etc.).

Use letters to identify the variants of the protocol (e.g. a, b, ...). A new variant is the same protocol version with different variations in the procedure (e.g. the same protocol with a change in the instrument settings, different volumes used, etc.).

Brief description:

Long description:

References:

Development phase:

Training purpose

Confidentiality:

License:

If the protocol is Open Access, please select one option from the Creative Commons copyright licenses.

Contacts

Name and email of contact person for the protocols:

 First name * Last name * Email *

Technique and Endpoints

In the lists below mark techniques and endpoints for which this protocol can be used.

(List of endpoints and techniques covered by the ACEnano project).

Techniques:

- Assay-on-a-chip
- Asymmetrical field flow fractionation
- Atomic Force Microscopy
- Brunauer–Emmett–Teller analysis
- Capillary electrophoresis
- Centrifugal Field-Flow Fractionation-MALS
- Centrifugal field flow fractionation
- Column test
- Dialysis + ICP-MS

Hold down "Control", or "Command" on a Mac, to select more than one.

Endpoints:

- Average size dimension
- Batch dispersion / stability
- Crystalline phase
- Density
- Deposition rate
- Elemental composition and chemical purity
- Functional coating
- Homoaggregation rate
- Hydrophobicity

Hold down "Control", or "Command" on a Mac, to select more than one.

Part 2: Steps

Please provide details for each step (action) of your sample preparation protocol.

Step #: Action:

1	Suspension
---	------------

[List of actions with descriptions.](#)

Medium:

-----	-----
-------	-------

+ Add a new medium

Medium volume:

Volume units:

- or -

Medium weight:

Weight units:

Sample concentration within the medium:

-----	-----
-------	-------

Concentration units:

Start phase:

End phase:

Delete this step

Step #: Action:

-----	Vortexing
-------	-----------

[List of actions with descriptions.](#)

Speed:

Speed units:

Speed duration:

Duration units:

Start phase:

End phase:

Preview protocol

Submit protocol

Make more changes

Part 2: Equipment

Equipment

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

Name: <input type="text"/>	Model: <input type="text"/>	Instrument type: <input type="text"/>
-------------------------------	--------------------------------	--

Common instrument makes and models.

Software: <input type="text"/>	Software version: <input type="text"/>
-----------------------------------	---

Limit of detection upper: <input type="text"/>	Limit of detection lower: <input type="text"/>	Limit of detection unit: <input type="text"/>
---	---	--

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.

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 <input type="text"/>	Value <input type="text"/>	Unit <input type="text"/>	<input type="checkbox"/> delete
Setting <input type="text"/>	Value <input type="text"/>	Unit <input type="text"/>	<input type="checkbox"/> delete
Setting <input type="text"/>	Value <input type="text"/>	Unit <input type="text"/>	<input type="checkbox"/> 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: [*] <input type="text"/>	Units: <input type="text"/>	<input type="checkbox"/> 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: [*] <input type="text"/>	Common setting: <input type="text"/>	Units: <input type="text"/>	<input type="checkbox"/> Delete
---	---	--------------------------------	---------------------------------

[+ Add another quality parameter](#)

[Continue to next step](#)

Part 3: Steps

Protocol steps

Please provide details for each step (action) of your measurement protocol and equipment used.

Step #:*

0

Name:*

Description:*

Image (optional)

 Choose File No file chosen Caption delete Delete this step + Add another step Preview protocol Submit protocol Make more changes

Sample Analysis by UV-Vis

Measurement protocol

This protocol describes quantification of the extinction of light that is measured from the spectral pattern using absorbance.

UV-Vis refers to the ultraviolet to visible spectral region of light, the absorption of which is size dependent at the nanoscale. UV-Vis is therefore an ideal technique for the size characterisation of NP suspensions through absorbance at an appropriate wavelength. The settings defined below will be refined to optimise results during the subsequent runs.

Measurement

Endpoints	Average size dimension
Technique	Ultraviolet-visible spectroscopy (UV-Vis)
Type of raw data produced	- Absorption wavelength (λ) (nm) - Absorbance
Phase in which the measurement is performed	Aqueous liquid

Instruments

Instrument	UV-Vis Spectrometer		
Type of instrument	Jenway 6800		
Instrument model	Double Beam Spectrometer		
Settings and parameters	Setting	Value	Unit
Measurement Mode Spectrum Scan -			
Data Mode ABS -			
Start Wavelength 680 nm			
End Wavelength 380 nm			
Scan Speed 400 nm/min			
Sampling Interval 0.5 -			
Slit Width 1.5 -			
Path Length 10 -			
Software	Flight Deck - 1.0 & high		
Instrument	Calibrated Volume Pipettors		
Type of instrument	1 mL and 5 mL		
Instrument	Disposable tips		
Type of instrument	1 mL and 5 mL		

Steps

1 Switch on the spectrometer

Switch on the UV-Vis Spectrometer and leave for 20 minutes to allow the lamp to heat up.

2 Prepare reference sample

Use 18.2 MΩ·cm Ultrapure water as the reference sample

3 Set-up the instrument parameters

Before starting the measurements, the parameter settings should be set in the software (Flight Deck 1.0 or higher).

4 Baseline correction

Baseline correction should be obtained by running a baseline using two cuvettes filled with 1 mL of Ultrapure Water each, placed in the sample holders

5 Add the cuvette with the sample

The reference cuvette with 1 mL UPW should then be left untouched and the other cuvette should be replaced with a new cuvette containing 1 mL of one of the diluted AuNP suspensions. A new cuvette should be used for each different sample analysed.

6 Run the measurement on known samples

Three spectrum scan runs for each known BBI AuNP diluted suspension (5, 20, 40, 60 and 100 nm) should be obtained. Therefore a total of 15 scans should be collected. The results obtained should be reported as explained in data treatment protocol and a calibration curve should be plotted.

7 Run the measurement on unknown samples

Following this three spectrum scan runs for the unknown monodispersed AuNP suspension containing a mono-dispersed suspension of NPs of an unknown size.

Linked to datasets

Protocol development phase: Cross lab testing (WP2)
 Confidentiality: Restricted Access only to ACEnano project members
 Organisation: UoB - The University of Birmingham
 Project: ACEnano - Analytical and Characterisation Excellence in nanomaterial risk assessment: A tiered approach
 Protocol version: 1
 Protocol variant: a
 Original protocol name: Ultraviolet-visible Light Spectroscopy (UV-Vis)
 ACEnano ID: Ultraviolet-visible Light Spectroscopy (UV-Vis)

Discussions

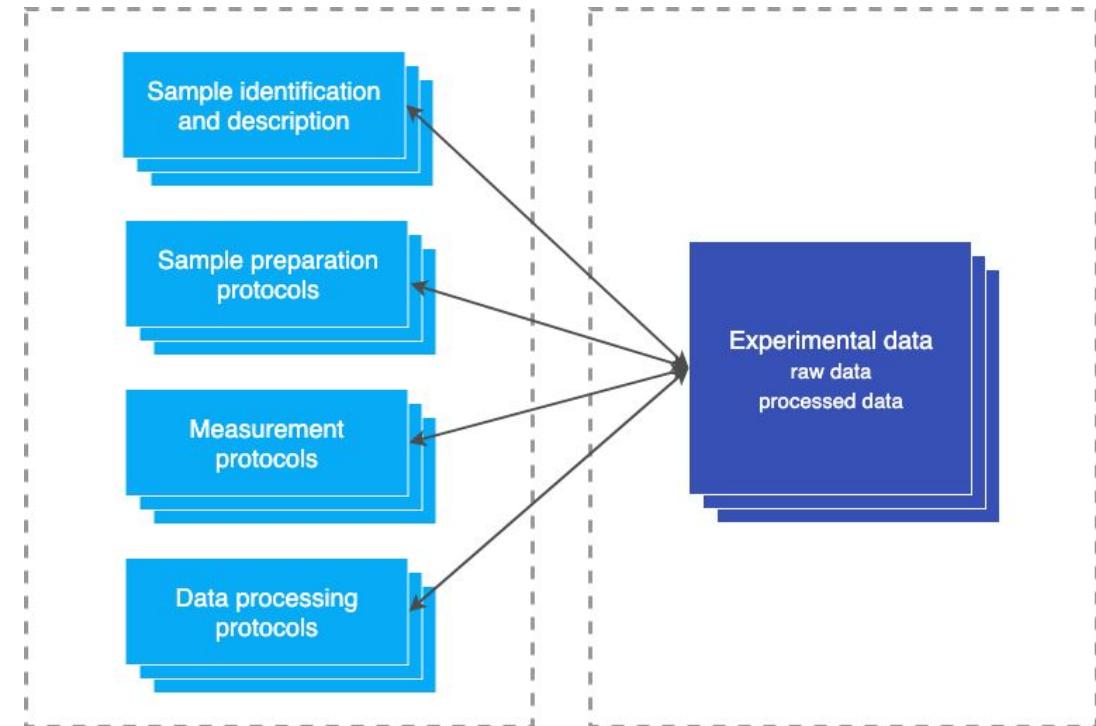
Questions?

Give us feedback: <https://it.research.net/r/calibrateusertesting>

Hands-on session: 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.



1

Technique and Endpoints

In the lists below mark techniques and endpoints for which this analysis was done.

([List of endpoints and techniques](#) covered by the ACEnano project).

Technique:*

Ultraviolet-visible spectroscopy

Endpoints:*

Homoaggregation rate

Hydrophobicity

Isoelectric Point

NP-cell interaction

Particle Size Distribution

Particle number concentration

Particle shape

ROS generation

Redox speciation

Hold down "Control", or "Command" on a Mac, to select more than one.

2

Protocols

Select a sample preparation protocol if one was used as part of your analysis.

Sample preparation protocol:

Continue to next step

3

Protocols

Select the measurement protocol used in your analysis.

Measurement protocol:

Continue to next step

4

Protocols

Select the data treatment protocol if one was used as part of your analysis.

Data treatment protocol:

Continue to next step

Select a protocol for preview

5

General information

Organisation submitting the analysis:

EwC - Edelweiss Connect GmbH

Analysis name:*

Brief description:

Long description:

References:

Confidentiality:*

License:

If the information and data provided are Open Access, please select one option from the [Creative Commons copyright licenses](#).

Contacts

Name and email of contact person for the analysis:

6

Sample description

Sample

Name*:

Code:

Supplier:

Batch number:

Sample phase:

Medium:

+Add a new medium

Sample volume:

Volume units:

Sample weight:

Weight units:

Concentration of material in sample:

Concentration units:

Nanoparticles in sample

Name: CAS number:

Coating: Crystalline phase: Shape:

Size: Size units:

Surface area: Surface area units:

Coating thickness: Units:

Delete this nanoparticle

+ Add nanoparticle



7

Data files

Dataset type: Raw	Dataset name: <input type="text"/>	Upload dataset: <input type="button" value="Choose File"/> No file chosen
<input type="checkbox"/> Delete this dataset		
Dataset type: Processed	Dataset name: <input type="text"/>	Upload dataset: <input type="button" value="Choose File"/> No file chosen
<input type="checkbox"/> Delete this dataset		
+ Add dataset		
Submit your data		

Analysis

Technique	Organisation	Filter	Reset
Characterisation of gold nanoparticles			
Technique: Ultraviolet-visible spectroscopy			
Endpoint: Average size dimension			
ACEnano_UVVis_Raw data_AuNP 20190605			
Raw			5 Jun 2019
ACEnano_UVVis_Results_AuNP 20190605			
Processed			
Particle Size Distribution by UV-Vis 20190603			
Technique: Ultraviolet-visible spectroscopy			
Endpoint: Particle Size Distribution			
Particle size distribution test 20190603			
Raw			3 Jun 2019
Particle size distribution test 20190603			
Raw			

View complete workflow

Characterisation of gold nanoparticles

This workflow describes the sample preparation, measurement and data treatment procedures for particle size measurements of gold NP suspensions. The procedure involves quantification of the extinction of light that is measured from the spectral pattern using absorbance. UV-Vis refers to the ultraviolet to visible spectral region of light, the absorption of which is size dependent at the nanoscale. UV-Vis is therefore an ideal technique for the size characterisation of NP suspensions through absorbance at an appropriate wavelength. The settings defined below will be refined to optimise results during the subsequent runs.

Technique: Ultraviolet-visible spectroscopy
Endpoints: Average size dimension

Datasets

- ACEnano_UVVis_Raw data_AuNP 20190605 - raw
- ACEnano_UVVis_Results_AuNP 20190605 - processed

Sample description

Name: Gold nanoparticles
Code: AuNP BBI Unknown
Supplier: BBI Solutions OEM Ltd
Medium: Unknown
Phase: Aqueous liquid
Sample volume: 1 mL
Concentration of material in sample: 50 mg/L

Nanoparticle

Core chemistry: Au
CAS number: 7440-57-5
Size: Unknown nm

Sample preparation protocol

For technique: Ultraviolet-visible spectroscopy
For endpoints: Average size dimension, Particle Size Distribution

- Vortexing** Mixing and dispersing of nanoparticles that are suspended in a liquid phase
Speed: /
Duration: 2 min
Phase change: Aqueous liquid → Aqueous liquid
- Dilution** Additional dilution of original sample for analysis

Data - view, filter, analyse, API

EdelweissData™ Explorer

Showing: 6 of 6 rows

Technique	Endpoint	Endpoint measure	Phase in which the measure...	Instrument	Type of instrument	Software version
Ultraviolet-visible spectrophot...	Particle size distribution	Absorption	Aqueous liquid	UVVis Spectrometer	Jenway 6800	Flight Deck - 1.0
Ultraviolet-visible spectrophot...	Particle size distribution	Absorption	Aqueous liquid	UVVis Spectrometer	Jenway 6800	Flight Deck - 1.0
Ultraviolet-visible spectrophot...	Particle size distribution	Absorption	Aqueous liquid	UVVis Spectrometer	Jenway 6800	Flight Deck - 1.0
Ultraviolet-visible spectrophot...	Particle size distribution	Absorption	Aqueous liquid	UVVis Spectrometer	Jenway 6800	Flight Deck - 1.0
Ultraviolet-visible spectrophot...	Particle size distribution	Absorption	Aqueous liquid	UVVis Spectrometer	Jenway 6800	Flight Deck - 1.0
Ultraviolet-visible spectrophot...	Particle size distribution	Absorption	Aqueous liquid	UVVis Spectrometer	Jenway 6800	Flight Deck - 1.0

Showing: 6 of 6 rows

Start Wavelength	End Wavelength	Sample name	Sample code	Supplier	Phase	Core chemistry
680 nm	380 nm	Gold nanoparticles	AuNP 5 nm	BBI Solutions OEM Ltd	Aqueous liquid	Au
680 nm	380 nm	Gold nanoparticles	AuNP 20 nm	BBI Solutions OEM Ltd	Aqueous liquid	Au
680 nm	380 nm	Gold nanoparticles	AuNP 40 nm	BBI Solutions OEM Ltd	Aqueous liquid	Au
680 nm	380 nm	Gold nanoparticles	AuNP 60 nm	BBI Solutions OEM Ltd	Aqueous liquid	Au
680 nm	380 nm	Gold nanoparticles	AuNP 100 nm	BBI Solutions OEM Ltd	Aqueous liquid	Au
680 nm	380 nm	Gold nanoparticles	AuNP BBI Unknown	BBI Solutions OEM Ltd	Aqueous liquid	Au

EdelweissData™

Size	Size unit	Stock concentration	Stock concentration unit	Max absorption wavelength	Absorbance	Measured size
5	nm	50	mg/L	547	0.402	
20	nm	50	mg/L	524	0.501	
40	nm	50	mg/L	530	0.547	
60	nm	50	mg/L	534	0.666	
100	nm	50	mg/L	571	0.47	
Unknown	nm	50	mg/L	548	0.719	78

Discussions and conclusions for the day

Questions?

Give us feedback: <https://it.research.net/r/calibrateusertesting>



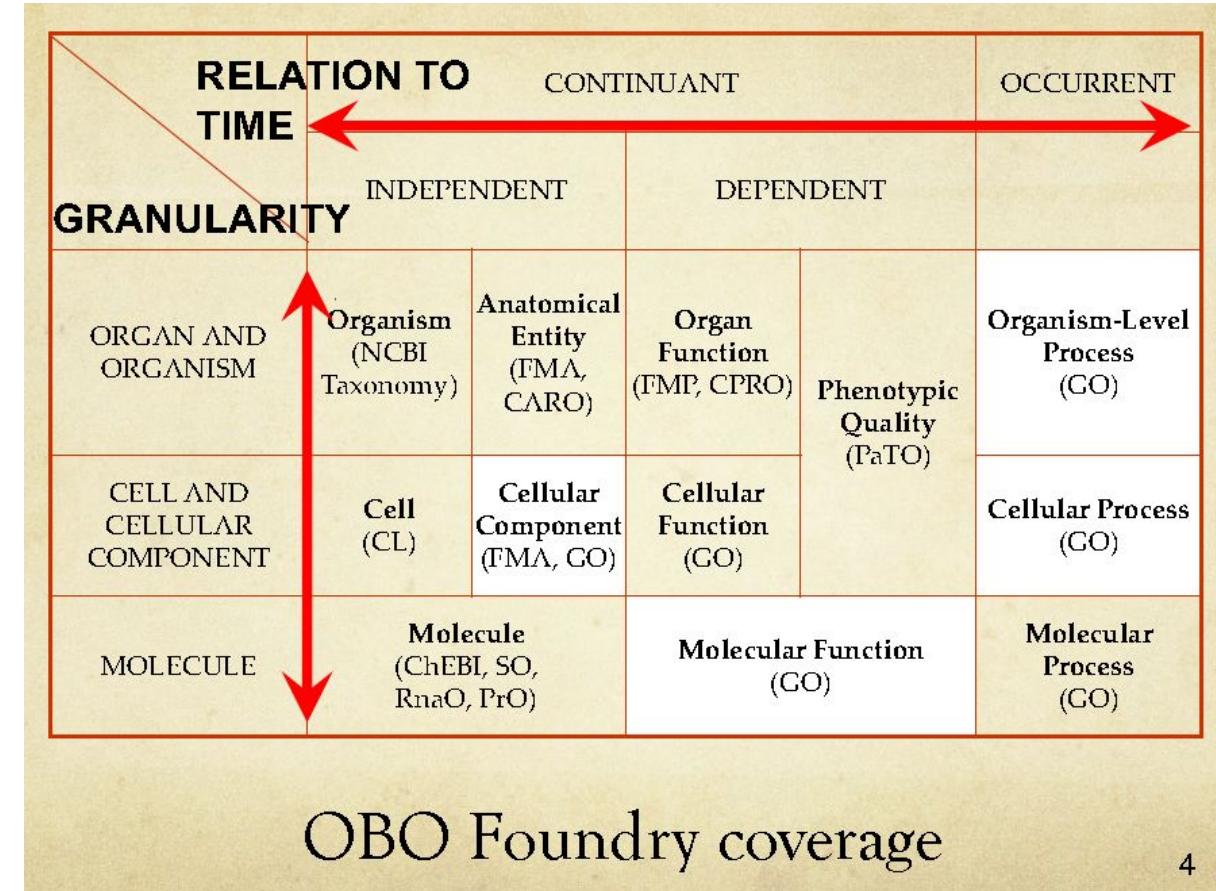
Analytical and Characterisation Excellence in nanomaterial risk assessment: A tiered approach

Thank you for your attention!

Introduction to the annotations / ontology topic

- Evolved from the interoperability requirement for system integration
 - data heterogeneity
 - semantic heterogeneity
- An ontology is a **data model that represents a domain** and is used to reason about the objects in that domain and the relations between them
- An ontology is a (partial) **specification of a shared conceptualization**, i.e., it is usually a logical theory that expresses the conceptualization explicitly in some language. A conceptualization can be defined as an intensional semantic structure that **encodes implicit knowledge** constraining the structure of a piece of a domain.

The use of ontologies began in the **biological sciences** around 1998 with the development of the Gene Ontology (GO). By 2007, there was sufficient interest and activity in the area to merit **national and international coordination efforts** such as the Open Biomedical Ontologies (OBO) Foundry or the National Center for Biomedical Ontologies.



The backbone of ontology is often a taxonomy.

Taxonomy is a classification of things in a hierarchical form. It is usually a tree or a lattice that expresses subsumption relation - i.e., A subsumes B meaning that everything that is in A is also in B.

An example is classification of living organisms.

eNanoMapper
Last uploaded: September 27, 2018

Summary Classes Properties Notes Mappings Widgets

Jump to:

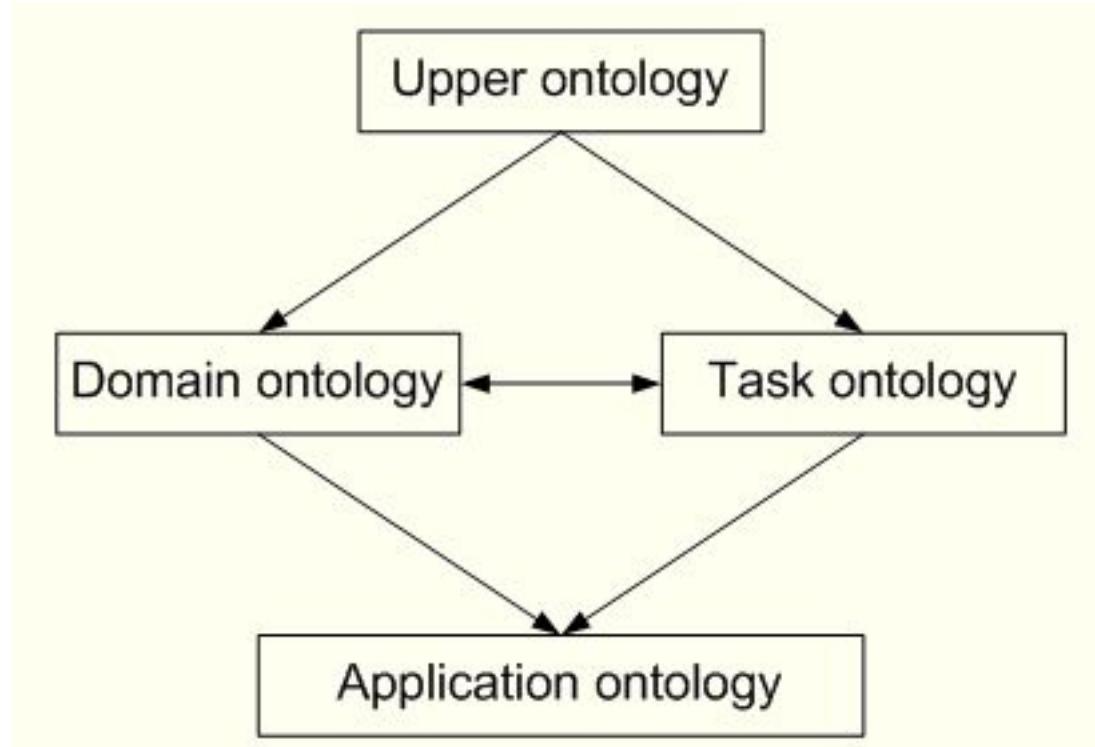
- entity
 - + disposition
 - + information content entity
 - + material entity
 - + process
 - quality
 - age
 - boiling point
 - chemical substance quality
 - concentration of dustiness
 - hydrodynamic size
 - intensity
 - mass
 - mass density
 - molecular entity quality
 - particle size
 - physical state
 - polydispersity
 - porosity
 - pour density
 - qualitative
 - rate
 - shape
 - size**
 - + solubility
 - Stability
 - surface area

Details Visualization Notes (0) Class Mappings (89) ⚙

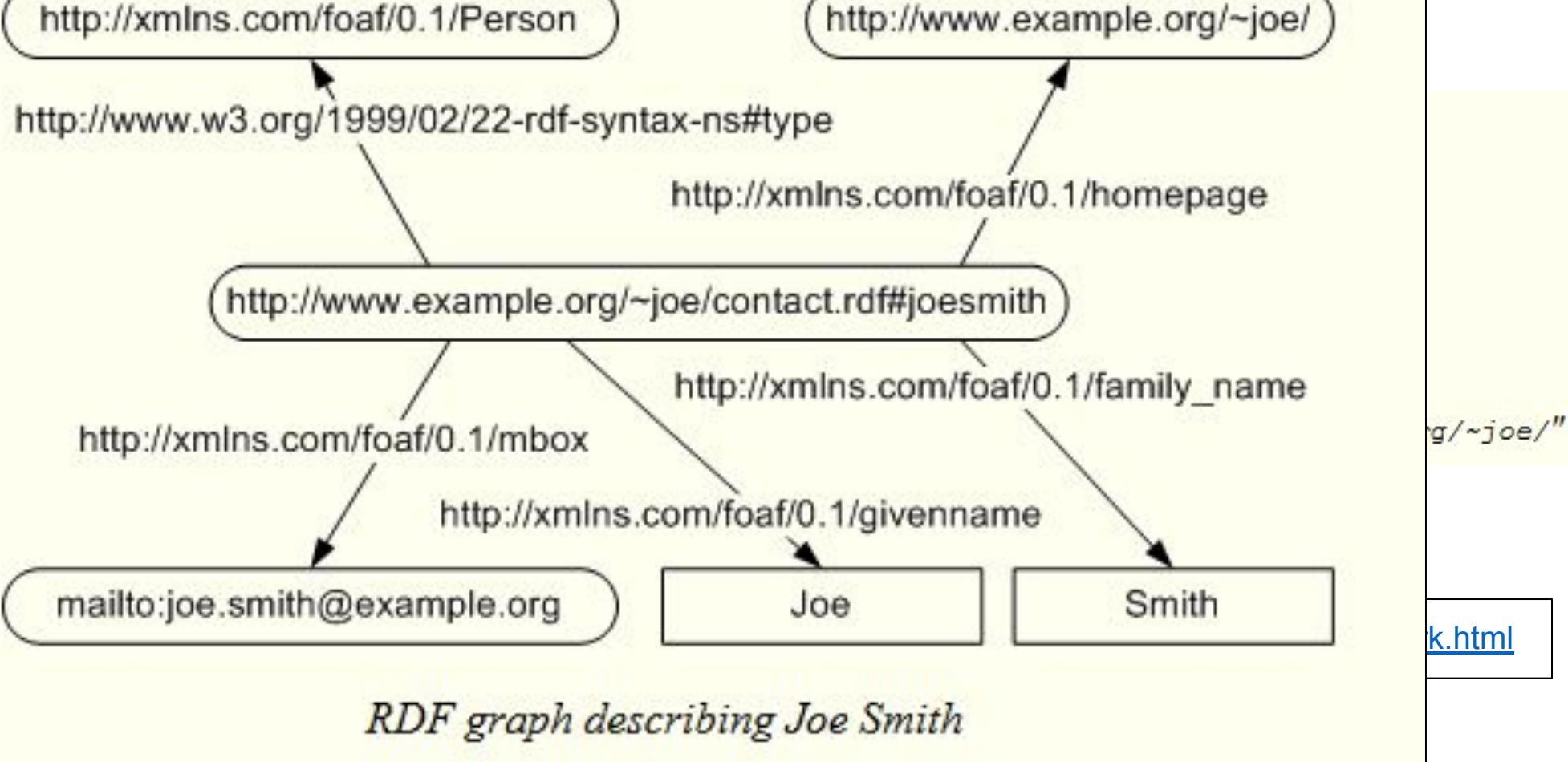
Preferred Name	size
Definitions	A morphology quality inhering in a bearer by virtue of the bearer's physical magnitude.
ID	http://purl.obolibrary.org/obo/PATO_0000117
has_obo_namespace	quality
id	PATO:0000117
in_subset	http://purl.obolibrary.org/obo/pato#scalar_slim http://purl.obolibrary.org/obo/pato#attribute_slim
label	size
notation	PATO:0000117
prefLabel	size
textual definition	A morphology quality inhering in a bearer by virtue of the bearer's physical magnitude.
subClassOf	quality

The modular design uses inheritance of ontologies

- upper ontologies describe general knowledge
- application ontologies describe knowledge for a particular application



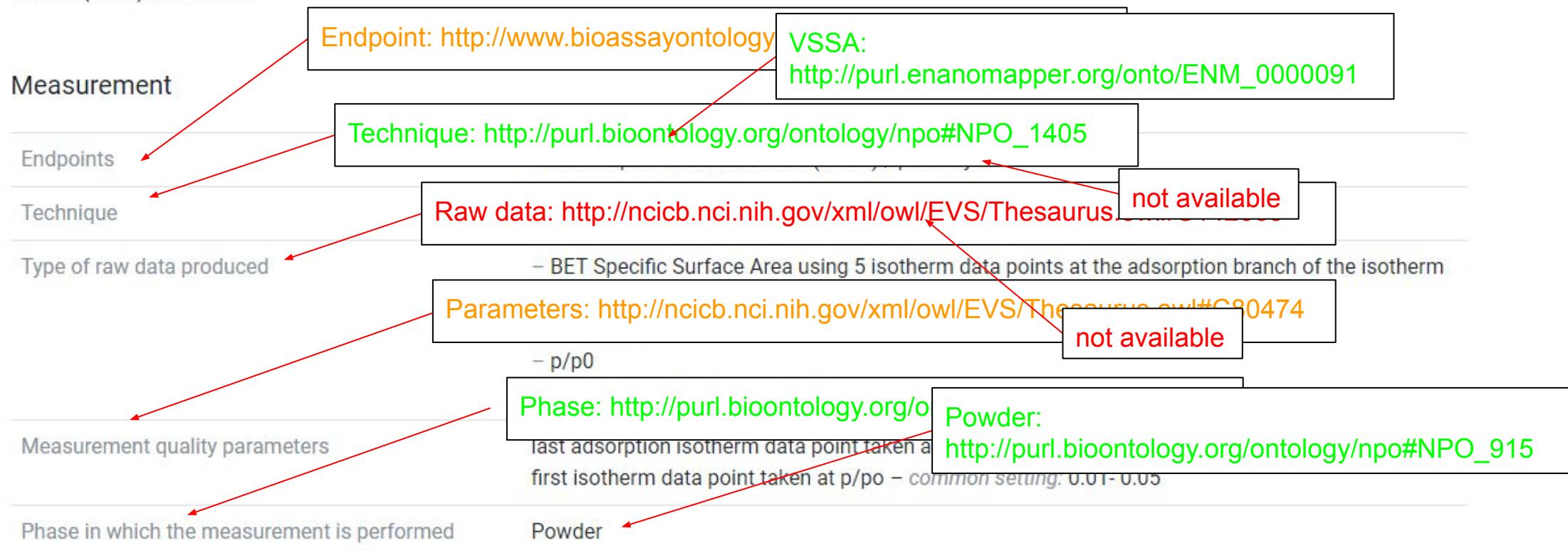
Resource Description Framework (RDF) is a framework for representing information about resources in a graph form.



Sample Analysis BET UoB test

Measurement protocol

This protocol describes the measuring of the amount of physically adsorbed gas according to the Brunauer, Emmett and Teller (BET) method.



Instrument

Instrument: http://purl.bioontology.org/ontology/npo#NPO_1436

Instrument

Parameters: <http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C80474>

Settings and parameters

not available

Setting	Value	Unit
N2	1.5	bar
He (or other inert gas in use)	2.0	bar
Warming time	20	min

Upper limit of detection

200 mg

Lowest limit of detection

100 mg

Steps

Lowest limit of detection:
<http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C80474>

Warming time: not available
Time: http://www.ebi.ac.uk/efo/EFO_0000721
Minute: http://purl.obolibrary.org/obo/GO_0000031

- 1 Switch on the BET instrument and wait 20 minutes for it to warm up.

If needed, switch on the vacuum pump.

Collection of required new classes

Warehouse Term	Ontology URL	BioPortal Description	Comparation Descriptions	Specialists Description
Wide-Angle X-ray Scattering	http://purl.obolibrary.org/obo/CHMO_0000207	A method for determining structure by measuring the change in direction or energy of X-rays scattered by a sample at wide angles (>10 deg.). Wide-angle X-ray scattering is used for determining the structure of polymers.	Missing Specialist	NA
Conductivity	http://purl.obolibrary.org/obo/NCIT_C134263	A measure of the ion-facilitated electron current through a material.	Missing Specialist	NA
Extractant	NA	NA	Missing Specialist	NA
Ionic strength	http://purl.obolibrary.org/obo/NCIT_C52478	The weighted concentration of ions in solutions.	Missing Specialist	NA
Purity (resistivity)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C62352	A quantitative assessment of the homogeneity or uniformity of a mixture. Alternatively, purity refers to the degree of being free of contaminants or heterogeneous components.	Missing Specialist	NA
Viscosity	http://purl.obolibrary.org/obo/NCIT_C75912	The resistance of a liquid to sheer forces and flow.	Missing Specialist	NA
Limit of Quantification- must be added in KI! Or add "Lower limit of detection" to eNM?	http://purl.obolibrary.org/obo/CHMO_0002802	The smallest measure that can be quantified with reasonable certainty for a given analytical procedure.	Missing in KI	Limit of quantification is the value which gives you the lowest, reliable quantifiable amount of a compound
Upper limit of detection	NA	NA	Missing in BioPortal	The largest value measurable using a defined method
Density	http://purl.enanomapper.org/onto/ENM_0000084	ENM	Missing in BioPortal	Mass per unit of volume
Dilution scale factor	NA	NA	Missing in BioPortal	The degree to which the concentration of a analyte has been reduced. 2. We only use dilution factor
Drying	http://purl.bioontology.org/ontology/npo#NPO_1956	ENM	Missing in BioPortal	The removal of water or solvent from a sample by evaporation
Vortexing	http://purl.bioontology.org/ontology/npo#NPO_1952	ENM	Missing in BioPortal	The mixing of liquids to produce a more homogenous sample using cyclic motion to produce a vortex
Dilution	???	NA	Missing in BioPortal	Reduction in concentration of an analyte
Sonication	http://purl.bioontology.org/ontology/npo#NPO_1961	ENM	Missing in BioPortal	The use of sound energy typically ultra hgh frequency to agi or mix samples
Heating	http://purl.bioontology.org/ontology/npo#NPO_1958	ENM	Missing in BioPortal	Increasing temperature
Milling	???	NA	Missing in BioPortal	The use of rotational cutting or grinding to reduce the size o bulk material

https://docs.google.com/spreadsheets/d/1mqt4epvvXMDFjpO5KeY_2u135WFXAhJfEXY4mkZH-A/edit

Available terms often not specific enough or misleading

- More complex terms needed
- Better definitions
- More training

OpenRiskNet / home

Unwatch ▾ 20 Star 6 Fork 3

Code Issues 26 Pull requests 0 Projects 2 Wiki Insights

Modelling IC50 results

Tim Dudgeon edited this page on 18 Dec 2018 · 11 revisions

Edit New Page

At the OpenRiskNet Hackathon in Brussels on 13-14 Dec 2018 we undertook an exercise on how to model IC50 assay with Json Schema (with respect to OpenAPI definitions) and how to semantically annotate this using Json-LD. OpenAPI (along with Json schema) provides the structured definition of the data whilst Json-LD is used to add semantic meaning to this payload using ontologies.

Ontology IRIs needed

For:

- IC50 (in ENM, from BAO)
- hill model fitting (Hill equation in BAO; added)
- tcpl (too specific, won't do)

Pages 11

Find a Page...

Home

Annotating API to make it queryable

Annotating your service to make it discoverable

CI CD environment

Development Guidelines

Glossary

Brunauer-Emmett-Teller equation - Human Physiology Simulation Ontology (HUPSON)

http://scai.fraunhofer.de/HuPSON#SCAIVPH_00000105

An extension of the Langmuir isotherm equation in the study of sorption; used for surface area determinations by computing the monolayer area.

Abbreviated BET equation. source: ...

[details](#) - [visualize](#)

Jenkins

Jenkins > eNanoMapper >

BiGCaT
department of bioinformatics

Jenkins 4 BiGCaT

View of jobs that build the eNanoMapper ontology, used by NanoSafety Cluster projects, partly funded by the

All Cytoscape plugins GUI tests Monitoring and data integrity Open PHACTS PathVis

eNanoMapper

S	W	Name ↓	Last Success
●	●	eNanoMapper - AOP	6 hr 40 min - #8
●	●	eNanoMapper - BAO	6 hr 41 min - #4
●	●	eNanoMapper - BFO	6 hr 41 min - #3
●	●	eNanoMapper - CCONT	6 hr 35 min - #3
●	●	eNanoMapper - CHEBI	6 hr 40 min - #3
●	●	eNanoMapper - CHEMINF	6 hr 41 min - #3
●	●	eNanoMapper - CHMO	6 hr 35 min - #3
●	●	eNanoMapper - EFO	6 hr 35 min - #7
●	●	eNanoMapper - ENVO	6 hr 40 min - #3
●	●	eNanoMapper - FABIO	6 hr 34 min - #3
●	●	eNanoMapper - HUPSON	6 hr 34 min - #4
●	●	eNanoMapper - IAO	6 hr 34 min - #3

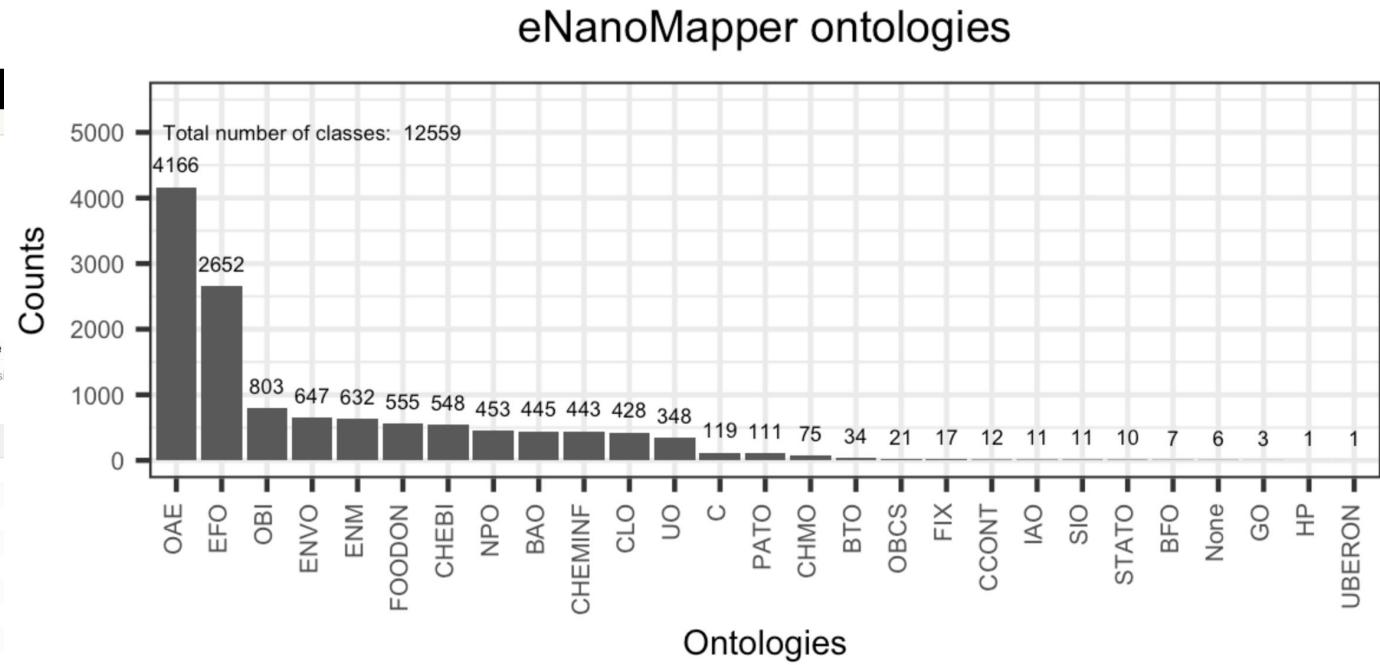
Build Queue
No builds in the queue.

Build Executor Status

master
1 Idle
2 Idle
3 Idle

calculation02-linux-highperformancememory

1 Idle
2 Idle



Releases after the management responsibility was transferred to NanoCommons:

5.0: 13 September 2018, 12,536 classes (update of CHEMINF)

5.0.1: 27 September 2018 (bug fixes)

5.0.2: 27 September 2018 (change in hosting)

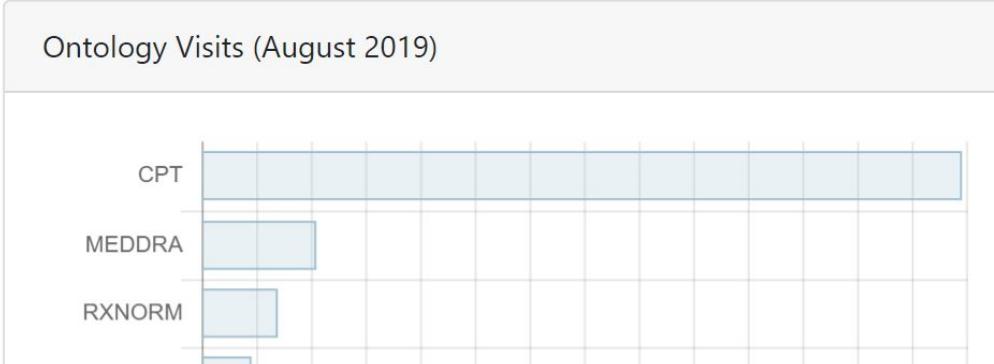
6.0: 30 August 2019, 12,732 terms (addition of OECD Testing Guidelines)

Provided by Egon Willighagen, UM

 BioPortal [Ontologies](#) [Search](#) [Annotator](#) [Recommender](#) [Mappings](#) [Resource Index](#) [Login](#)

Welcome to BioPortal, the world's most comprehensive repository of biomedical ontologies

Search for a class

 
[Advanced Search](#)

Find an ontology

 
[Browse Ontologies](#)

BioPortal Statistics

Ontologies	815
Classes	9,958,055
Resources Indexed	48

Description of techniques

Name:	Transmission Electron Microscopy
Name - Ontology URL:	Currently: http://purl.bioontology.org/ontology/npo#NPO_1430
	Change: http://purl.bioontology.org/ontology/npo#NPO_1430
Abbreviation:	TEM
Short description:	<p>Transmission electron microscopy (TEM, also sometimes conventional transmission electron microscopy or CTEM) is a microscopy technique in which a beam of electrons is transmitted through a specimen to form an image. The specimen is most often an ultrathin section less than 100 nm thick or a suspension on a grid. An image is formed from the interaction of the electrons with the sample as the beam is transmitted through the specimen. The image is then magnified and focused onto an imaging device, such as a fluorescent screen, a layer of photographic film, or a sensor such as a charge-coupled device.</p> <p>Source: https://en.wikipedia.org/wiki/Transmission_electron_microscopy</p>



Details		Visualization	Notes (0)	Class Mappings (35)	⊕
Preferred Name	transmission electron microscopy				
Synonyms	TEM technique				
Definitions	<p>A light source at the top of the TEM emits the electrons that travel through vacuum in the column of the microscope. Instead of glass lenses focusing the light in the light microscope, the TEM uses electromagnetic lenses to focus the electrons into a very thin beam. The electron beam then travels through the specimen you want to study. Depending on the density of the material present, some of the electrons are scattered and disappear from the beam. At the bottom of the microscope the unscattered electrons hit a fluorescent screen, which gives rise to a shadow image of the specimen with its different parts displayed in varied darkness according to their density. The image can be studied directly by the operator or photographed with a camera. [source: http://Nobelprize.org]</p> <p><ncicp:ComplexDefinition>&lt;ncicp:def-definition>An electron microscopy technique based on the use of transmission electron microscope.&lt;/ncicp:def-definition>&lt;/ncicp:ComplexDefinition></p>				
ID	http://purl.bioontology.org/ontology/npo#NPO_1430				
comment	<p>A light source at the top of the TEM emits the electrons that travel through vacuum in the column of the microscope. Instead of glass lenses focusing the light in the light microscope, the TEM uses electromagnetic lenses to focus the electrons into a very thin beam. The electron beam then travels through the specimen you want to study. Depending on the density of the material present, some of the electrons are scattered and disappear from the beam. At the bottom of the microscope the unscattered electrons hit a fluorescent screen, which gives rise to a shadow image of the specimen with its different parts displayed in varied darkness according to their density. The image can be studied directly by the operator or photographed with a camera. [source: http://Nobelprize.org]</p>				
code	NPO_1430				
definition	<ncicp:ComplexDefinition><ncicp:def-definition>An electron microscopy technique based on the use of transmission electron microscope.</ncicp:def-definition></ncicp:ComplexDefinition>				
label	transmission electron microscopy				
preferred_name	transmission electron microscopy				
prefixIRI	npo:NPO_1430				
synonym	TEM technique				
subClassOf	electron microscopy				

Description of endpoints

Name:	Particle Size Distribution
Name - Ontology URL:	Currently: http://purl.bioontology.org/ontology/npo#NPO_1699
	Change: http://purl.bioontology.org/ontology/npo#NPO_1699

Details		Visualization	Notes (0)	Class Mappings (16)	⊕
Preferred Name	particle size distribution				
Definitions	<p><ncicp:ComplexDefinition xmlns:ncicp="http://ncicb.nci.nih.gov/xml/owl/EVS/ComplexProperties.xsd#"><ncicp:def-definition>A size distribution inhering in particles.</ncicp:def-definition><ncicp:Definition_Review_Date>100430</ncicp:Definition_Review_Date><ncicp:def-source>NPO</ncicp:def-source><ncicp:Definition_Reviewer_Name>Dennis Thomas</ncicp:Definition_Reviewer_Name></ncicp:ComplexDefinition></p>				
ID	http://purl.bioontology.org/ontology/npo#NPO_1699				
code	NPO_1699				
definition	A size distribution inhering in particles.100430NPODennis Thomas				
label	particle size distribution				
preferred_name	particle size distribution				
prefixIRI	npo:NPO_1699				
subClassOf	size distribution				

Description of Sample

Nanoparticles in sample

Name:

titanium dioxide nano

titanium dioxide nanoparticle
response pathway

http://purl.obolibrary.org/obo/PW_0001437
A pathway triggered by exposure to titanium dioxide nanoparticle (nano-TiO₂). Nano-TiO₂ has a broad range of applications but studies indicate that under conditions of long and high dose exposure, it can exert cytotoxic and genotoxic effects. Nano-TiO₂ has been shown to induce inflammation, oxidative stress and MAP kinase activity.

titanium dioxide nanoparticles

http://purl.obolibrary.org/obo/XCO_0000339
Any condition in which the main

CAS number:

Crystalline phase:

Size units:

nano

nano

http://purl.obolibrary.org/obo/UO_0000300
A prefix in the metric system denoting a factor of 10 to the power of -9.

nanoliter

http://purl.obolibrary.org/obo/UO_0000102
A volume unit which is equal to one thousandth of one millionth of a liter or 10⁻⁹ L.

nanometer

http://purl.obolibrary.org/obo/UO_0000018
A length unit which is equal to one thousandth of one millionth of a meter or 10⁻⁹ m.

Addition of media or compounds during sample preparation

Add a new medium

Name:

PBS

PbSub2

http://purl.obolibrary.org/obo/IDOMAL_0001082

A secreted protein expressed in ookinete stage forming protein aggregates that are often associated with the actin cytoskeleton.

PBS buffer

http://purl.obolibrary.org/obo/MSIO_0000021

Phosphated buffer saline (PBS) buffer is a buffer which is a water-based salt solution containing disodium hydrogen phosphate, sodium chloride and, in some formulations, potassium chloride and potassium dihydrogen phosphate.

Compound name:

sodium ch

sodium chloride

http://purl.obolibrary.org/obo/CHEBI_65242

An inorganic sodium salt that has chlorate as the counter-ion. An oxidising agent, it is used for bleaching paper and as a herbicide. It is also used in the manufacture of dyes, explosives and matches.

sodium chlorite

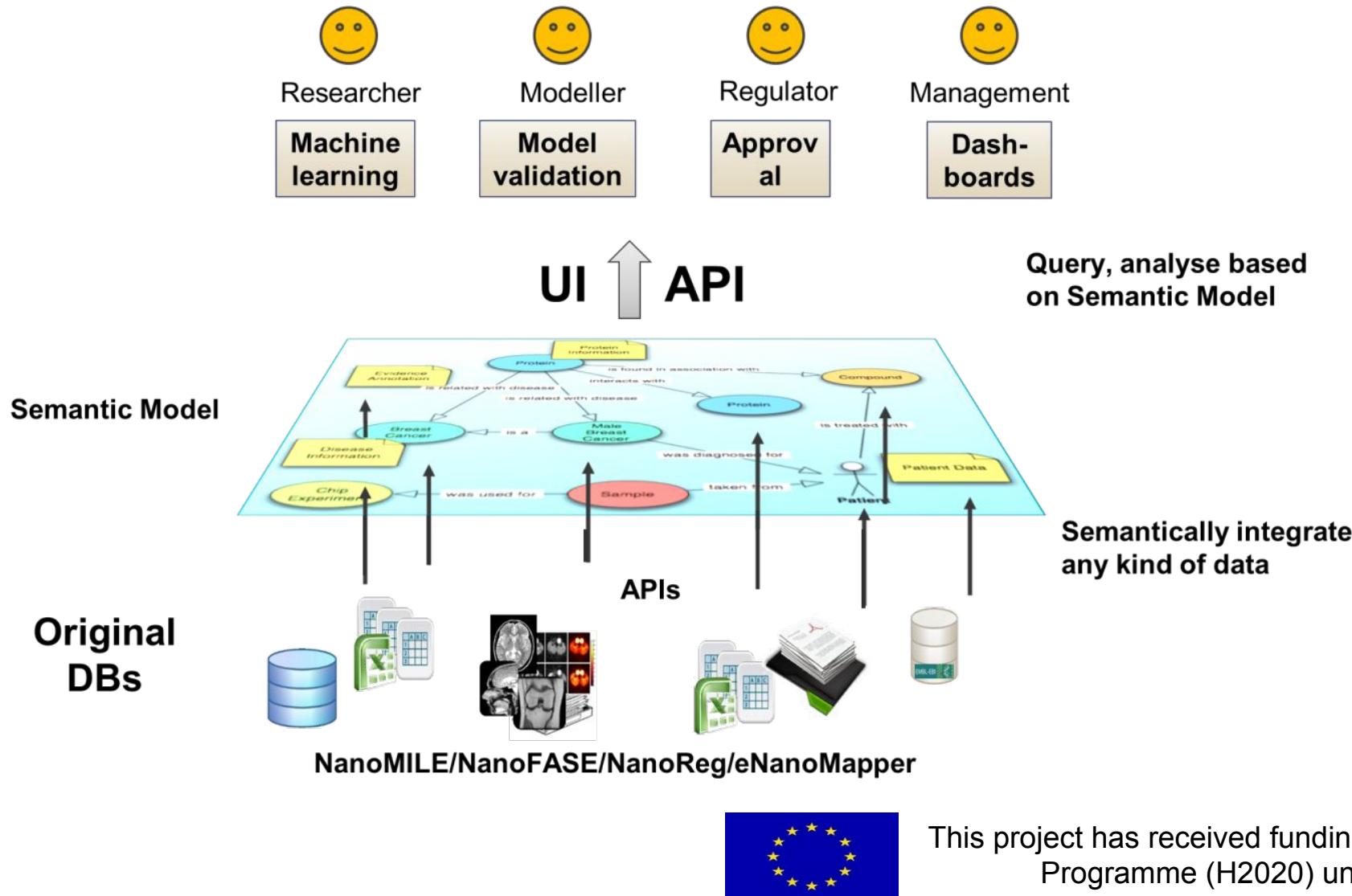
http://purl.obolibrary.org/obo/CHEBI_78667

An inorganic sodium salt in which chlorite is the counterion.

sodium chloride

http://purl.obolibrary.org/obo/CHEBI_26710

An inorganic chloride salt having



Public version provided and integrated by



NanoCommons

Nano-Knowledge Community

Hands-on session: protocols and data annotations

Term collection:

https://docs.google.com/spreadsheets/d/1mqt4epvvXMDFjpO5KeY_2u135WFXAhJfEXY4mkZH-A/edit

BioPortal for searching ontologies:

<https://biportal.bioontology.org/>

eNanoMapper ontology:

<https://enanomapper.net/ontology> and <https://biportal.bioontology.org/ontologies/ENM>