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

10 October 2019, Copenhagen, Denmark

Agenda

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	*Coffee break*
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

Objectives

- 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:

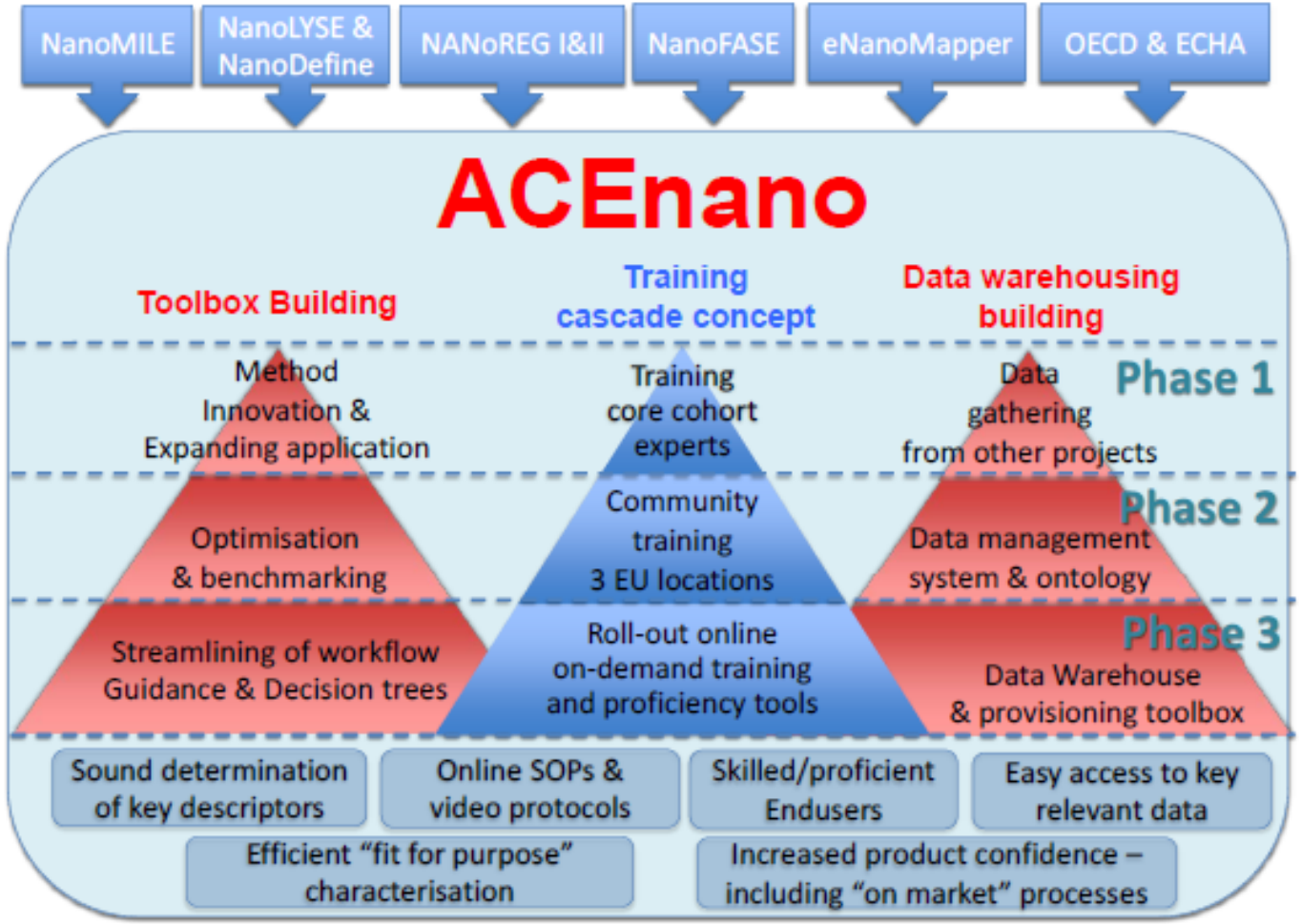
1. Add the sample preparation protocol
2. Add the measurement protocol
3. Add the data treatment protocol
4. Create the data workflow, including the description of the sample measured, and the protocols mentioned above
5. Upload raw and processed data files

Useful links and resources for participants:

- ACEnano Knowledge Infrastructure: https://acenano.douglasconnect.com/
- Knowledge Infrastructure Tutorial: https://github.com/NanoCommons/tutorials/tree/master/ACEnano_manuals
- 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**.



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

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

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

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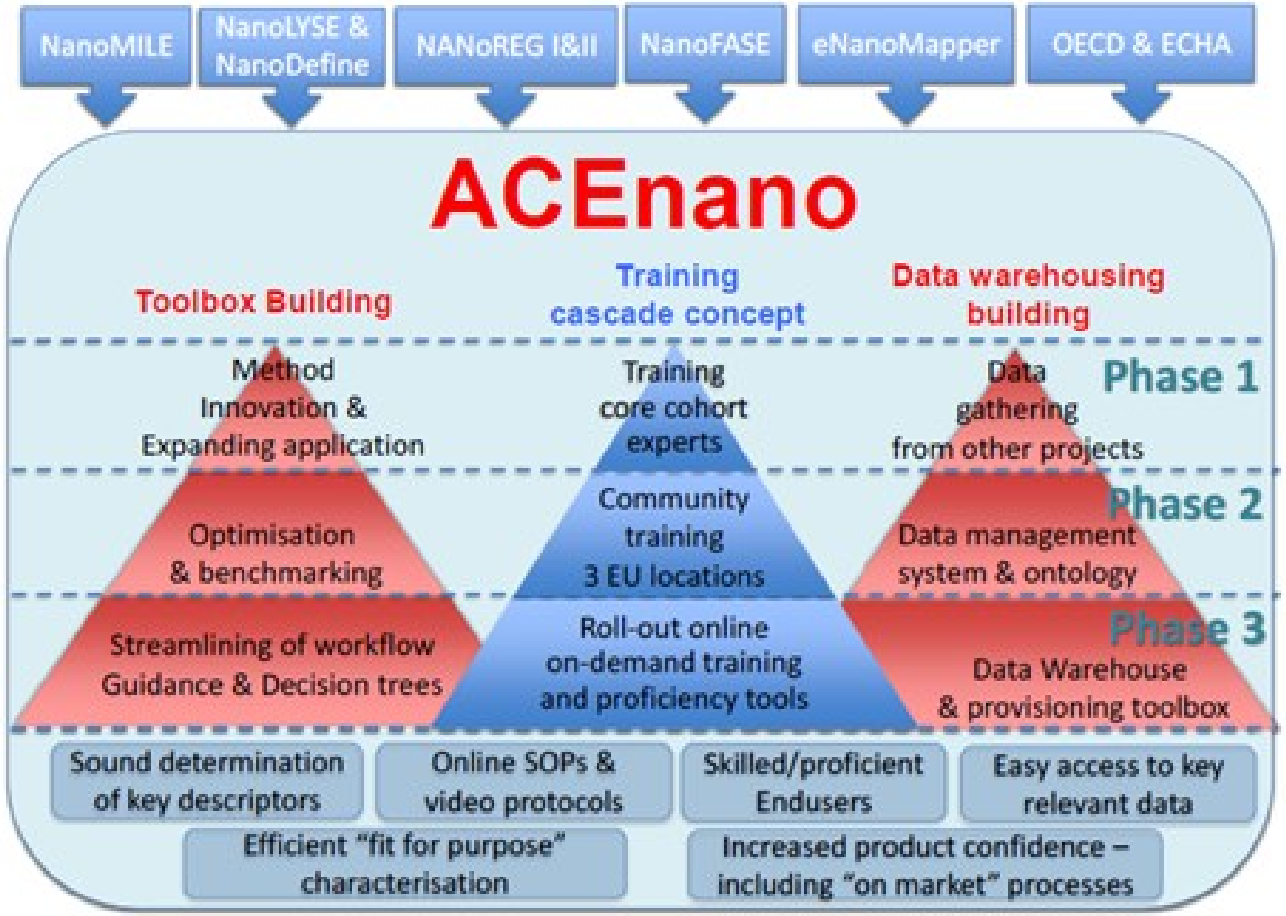
ACEnano

Analytical and Characterisation Excellence

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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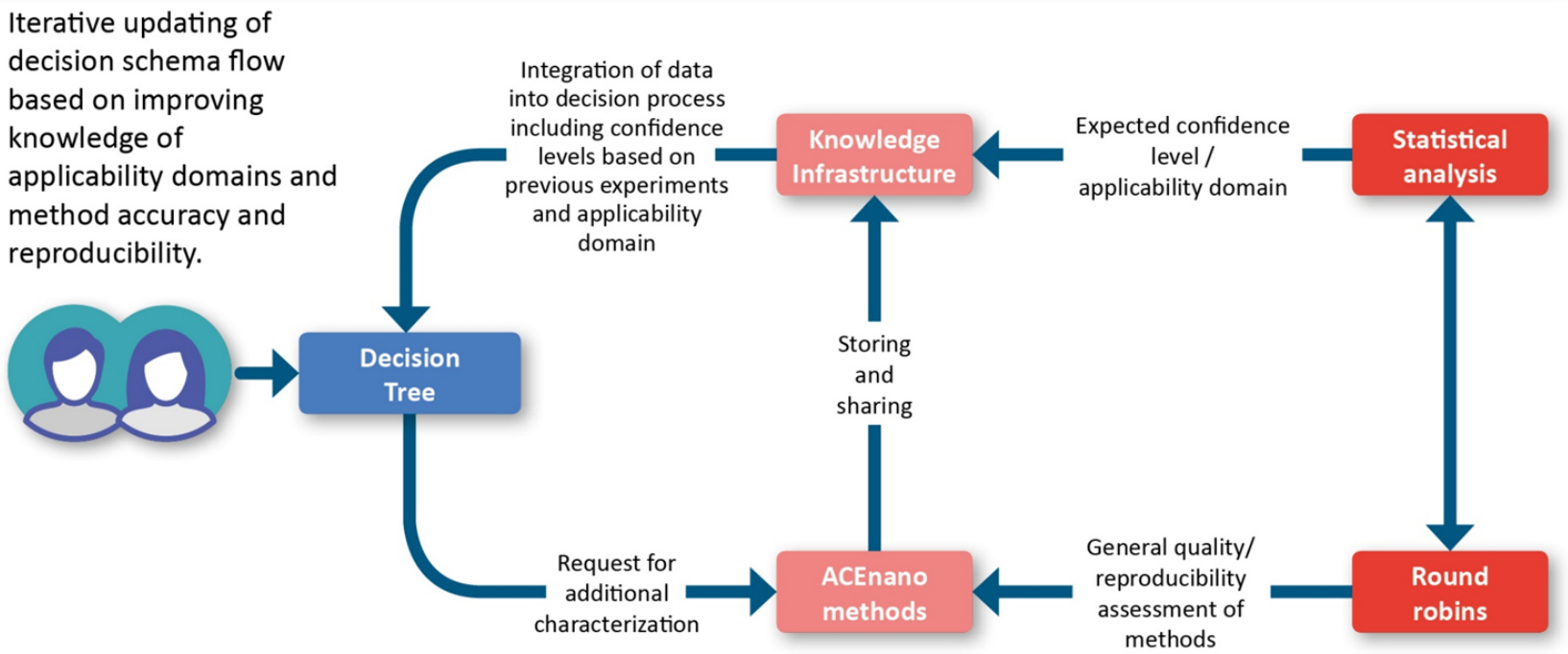
ACEnano
Analytical and Characterisation Excellence

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

Getting to efficient, cost-effective decisions on nanomaterial analysis



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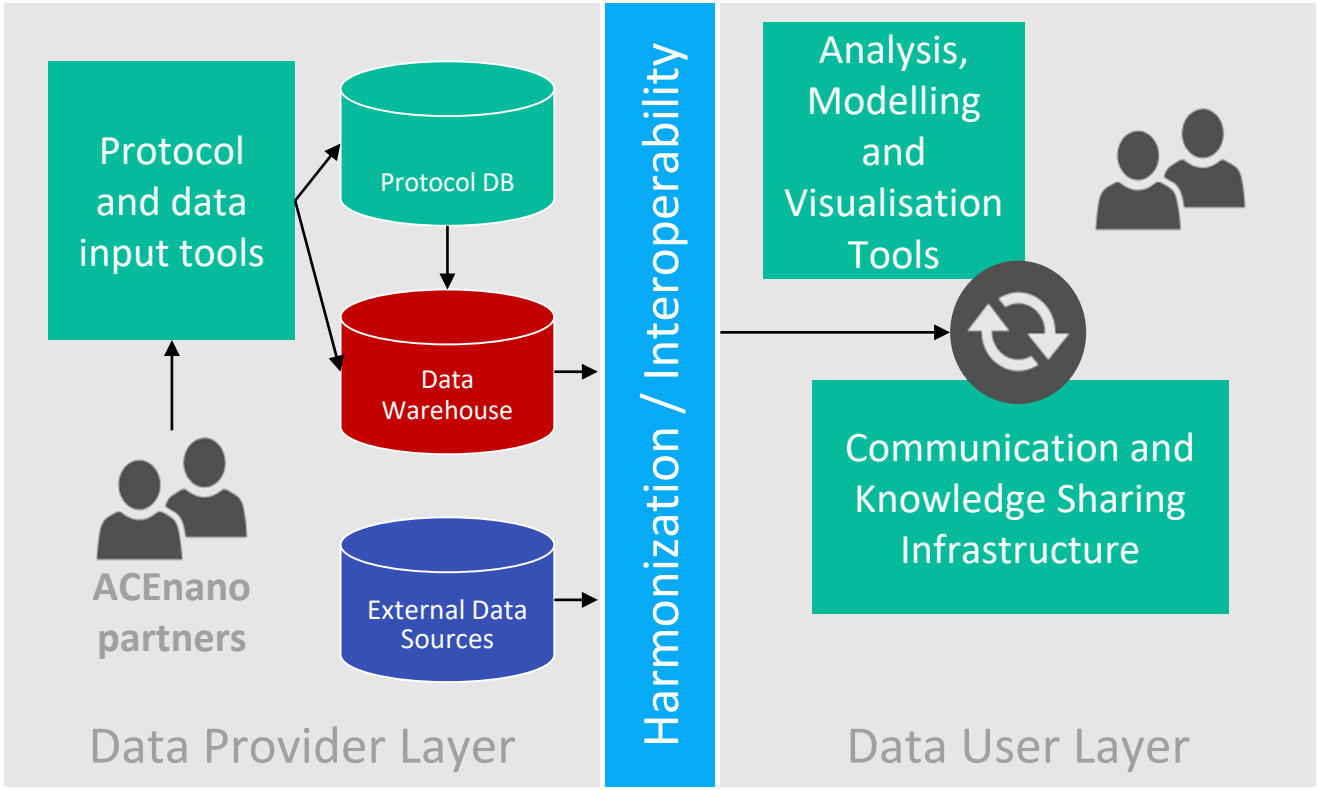
Analytical and Characterisation Excellence in nanomaterial risk assessment: A tiered approach



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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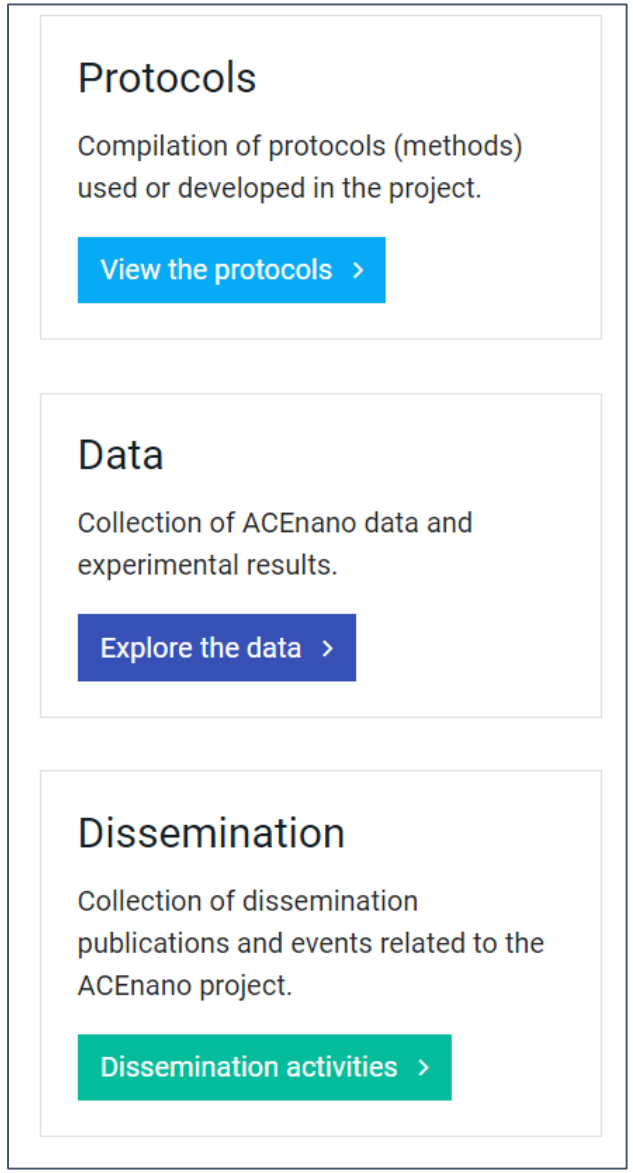
Introduction to the Knowledge Infrastructure

Data management approach

- 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

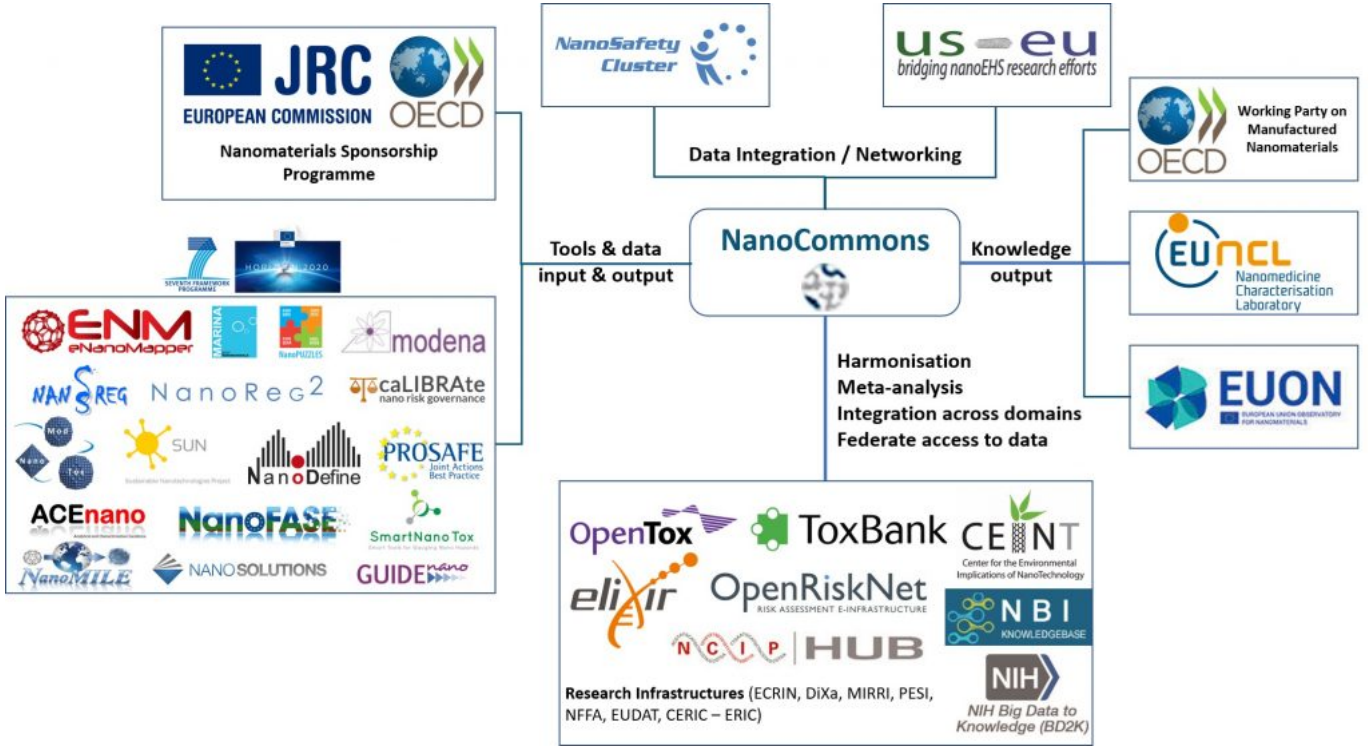
ACEnano Knowledge Infrastructure
https://acenano.douglasconnect.com/
A central platform to access harmonised and standardised methods applied for physicochemical characterisation of nanomaterials



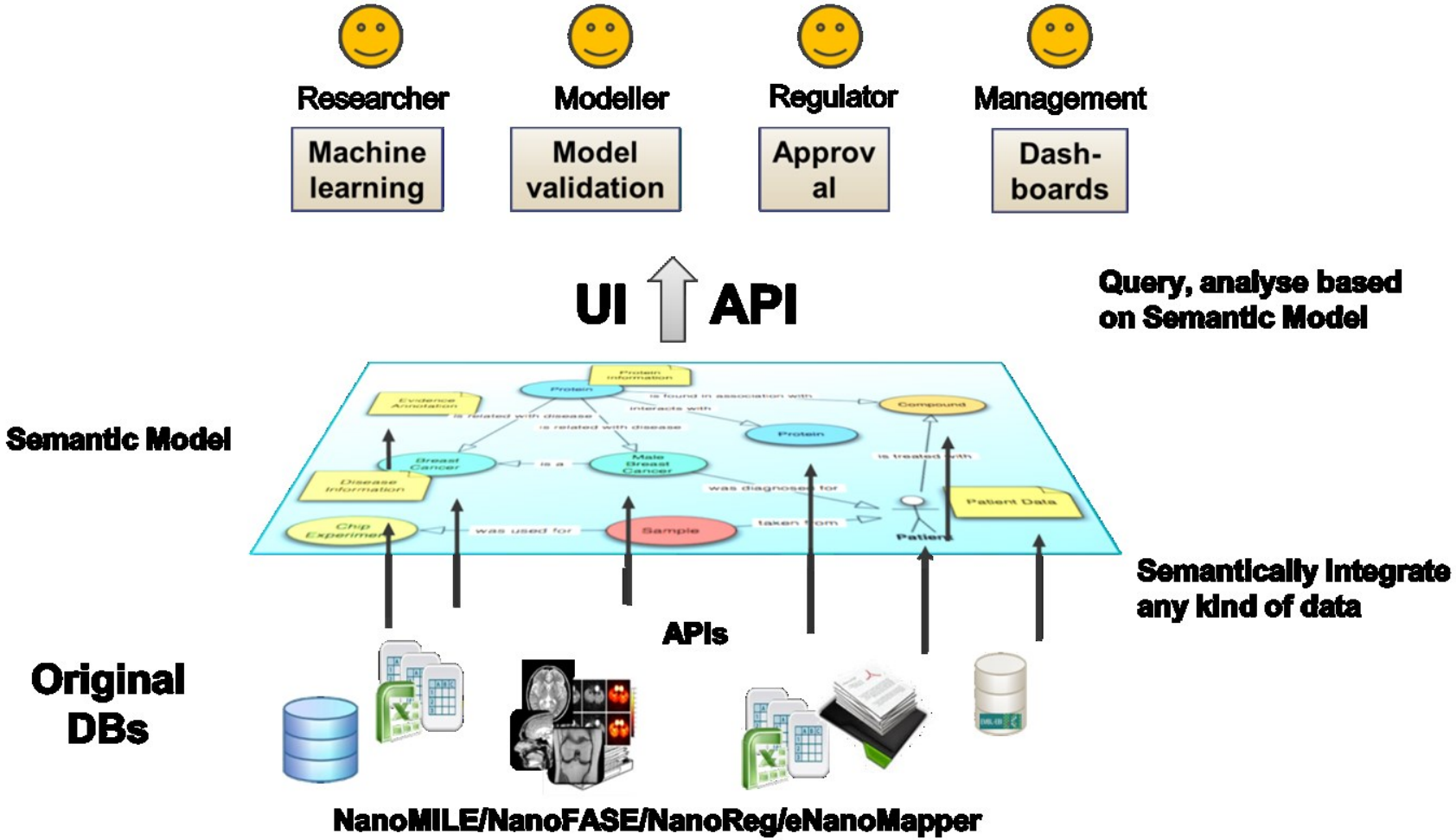
ACEnano
Analytical and Characterisation Excellence

NanoCommons
Nano-Knowledge Community

- **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.



Linking to other data sources



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

Semantic annotation

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.

Endpoint: http://www.bioassayontology

VSSA: http://purl.enanomapper.org/onto/ENM_0000091

Technique: http://purl.bioontology.org/ontology/npo#NPO_1405

not available

Raw data: http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus

Parameters: http://ncicb.nci.nih.gov/xml/owl/EVS/Th 0474

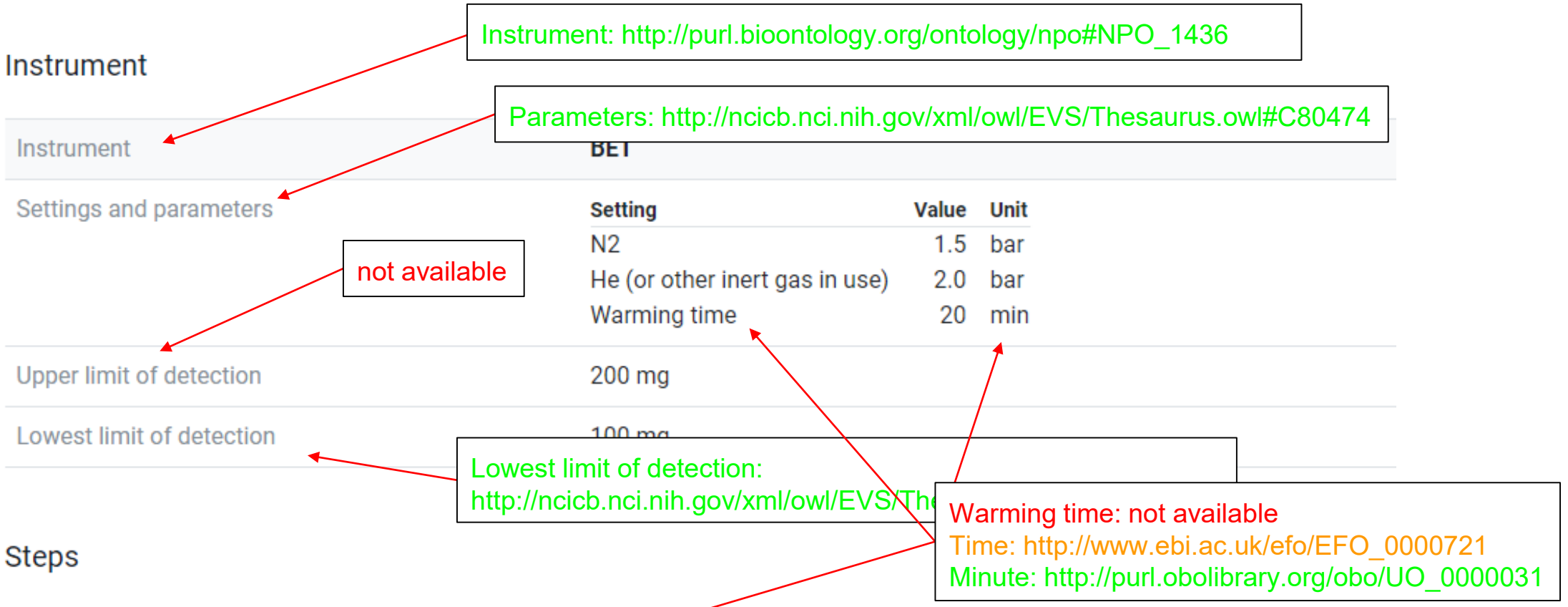
not available

Phase: http://purl.bioontology.org/o

Powder: http://purl.bioontology.org/ontology/npo#NPO_915

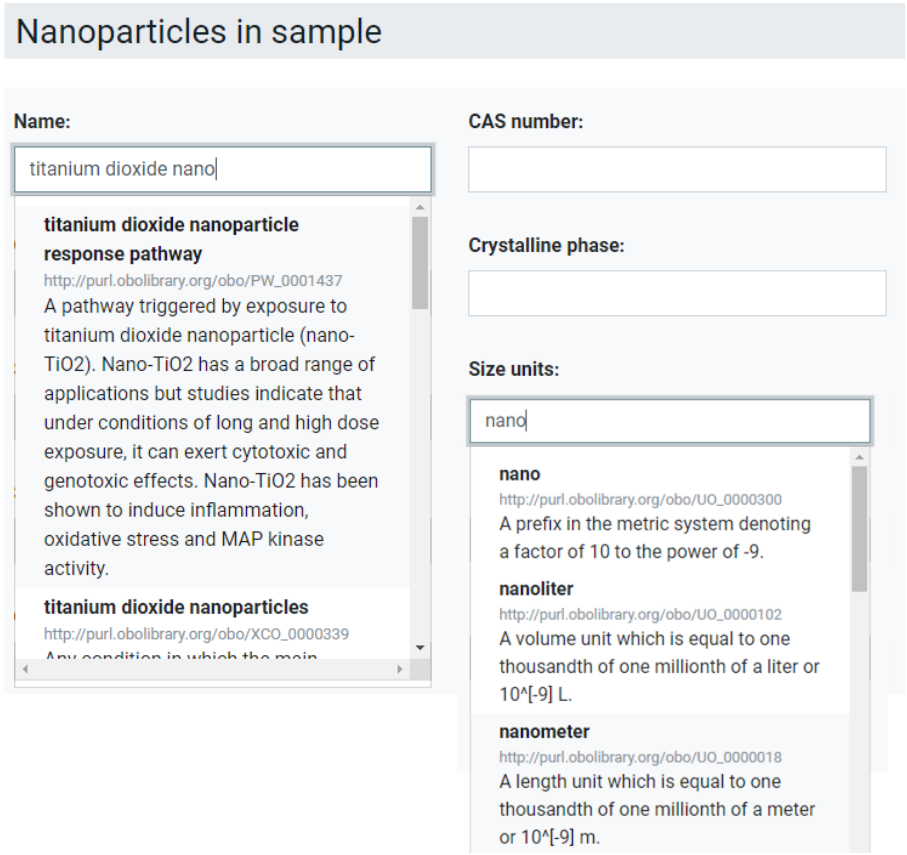
Measurement	
Endpoints	
Technique	
Type of raw data produced	– BET Specific Surface Area using 5 isotherm data points at the adsorption branch of the isotherm
Measurement quality parameters	– p/p0 last adsorption isotherm data point taken a first isotherm data point taken at p/po – *common setting:* 0.01- 0.05
Phase in which the measurement is performed	Powder

Semantic annotation

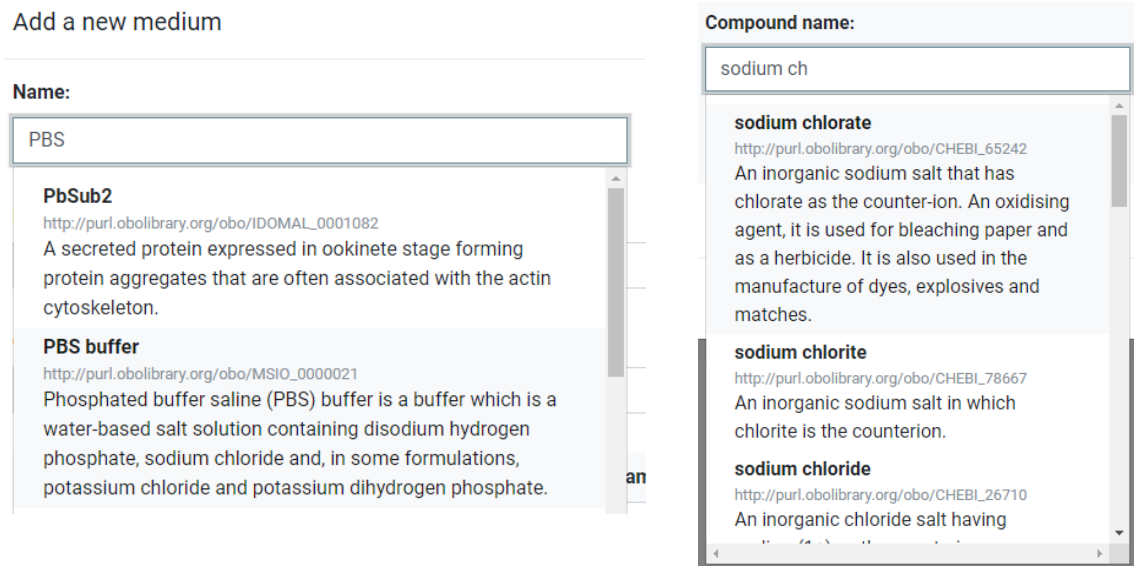


Ontology lookup service to support user input

Description of Sample



Addition of media or compounds during sample preparation



Collection of required new classes

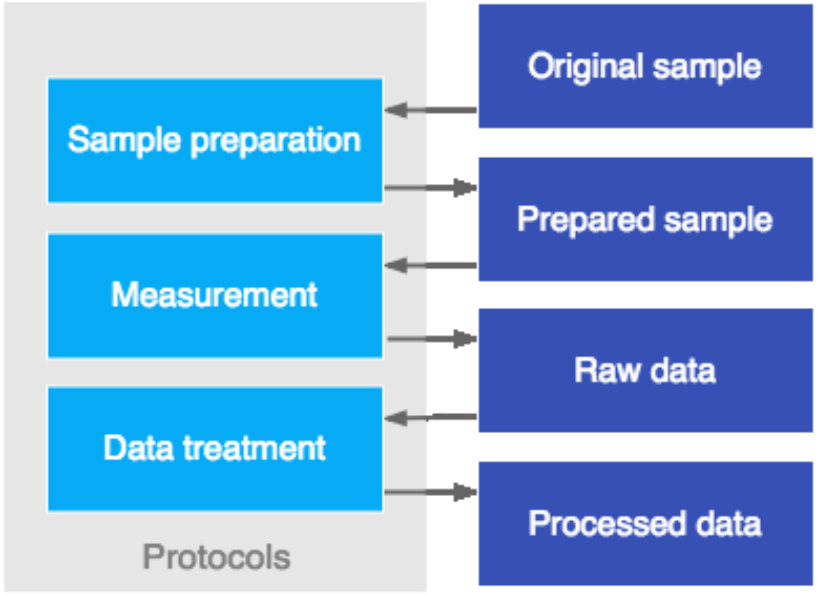
Warehouse Term	Ontology URL		BioPortal Description	Comparation Descriptions	Specialists Description
Wide-Angle X-ray Scattering	http://purl.obolibrary.org/obo/CHMO_0000207		A method for determining structure by measuring the change in direction or energy of X-rays scattered by a sample at wide angles (>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	NA	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 bee reduced, **2. We only use dilution factor**
Drying	http://purl.bioontology.org/ontology/npo#NPO_1956	ENM	NA	Missing in BioPortal	The removal of water or solvent from a sample by evaporati
Vortexing	http://purl.bioontology.org/ontology/npo#NPO_1952	ENM	NA	Missing in BioPortal	The mixing of liquids to produce a more homogenous sampl 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	NA	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	NA	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/1mqt4epvvXMDFjipO5KeY_2u135WFXAhJfEXY4mkZH-A/edit

Knowledge Infrastructure

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

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**	

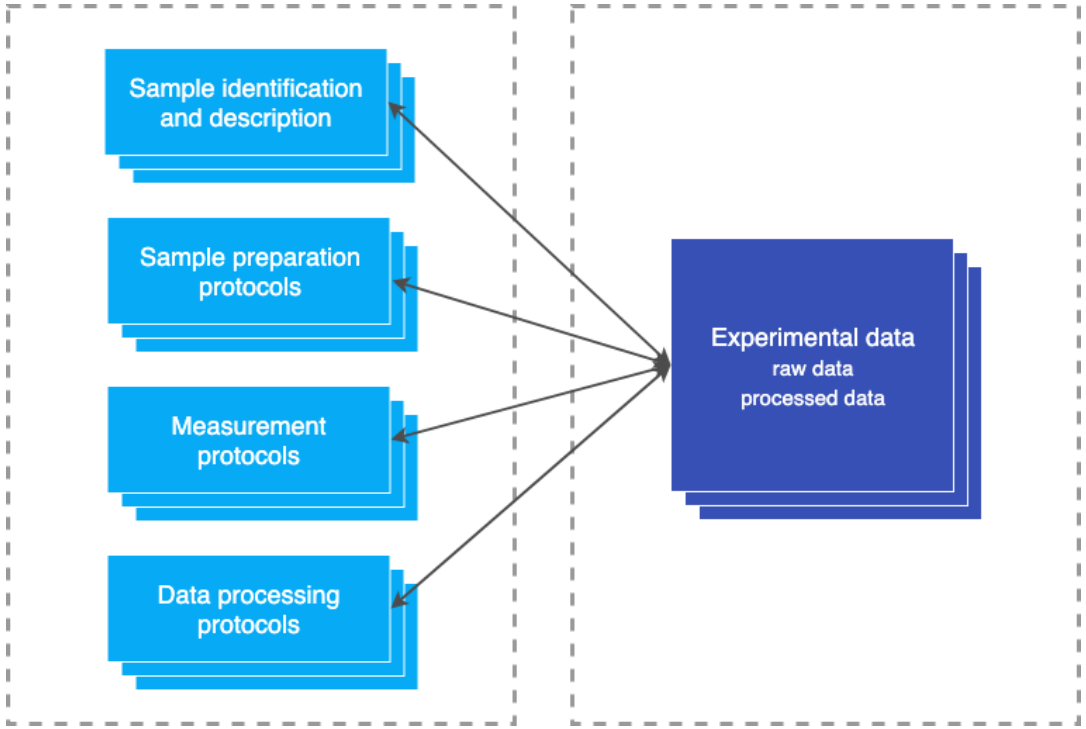
Data treatment protocol	
Part 1: General information	Protocol name and description
	Contacts
	Technique and Endpoints
Part 2: Steps	Steps and algorithm used
→ **Preview protocol, Make more changes & Submit protocol**	

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**	

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.



Data workflow and data upload

7

Data files

Dataset type:* Raw | **Dataset name:*** | **Upload dataset:*** Choose File No file chosen

Delete this dataset

Dataset type:* Processed | **Dataset name:*** | **Upload dataset:*** Choose File No file chosen

Delete this dataset

+ Add dataset

Submit your data

Technique | Organisation | Filter | Reset

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

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

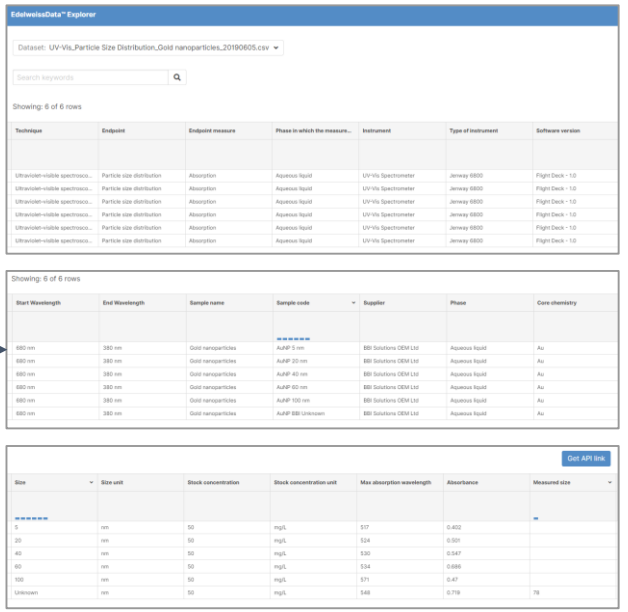
For technique: Ultraviolet–visible spectroscopy
For endpoints: Average size dimension, Particle Size Distribution

1 **Vortexing** Mixing and dispersing of nanoparticles that are suspended in a liquid phase

Speed:	/
Duration:	2 min
Phase change:	Aqueous liquid → Aqueous liquid

2 **Dilution** Additional dilution of original sample for analysis

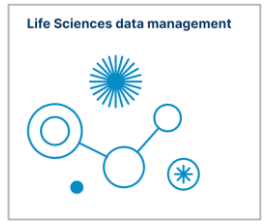
Data - view, filter, analyse, API

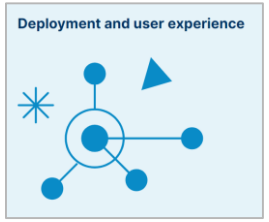


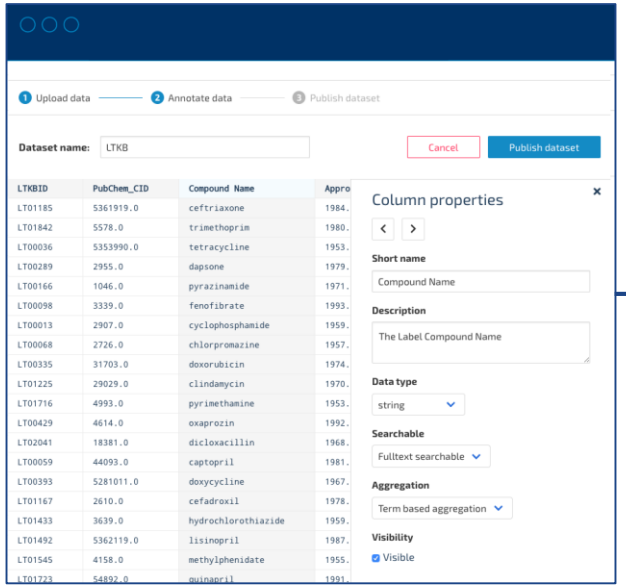
EdelweissData™

EdelweissData™

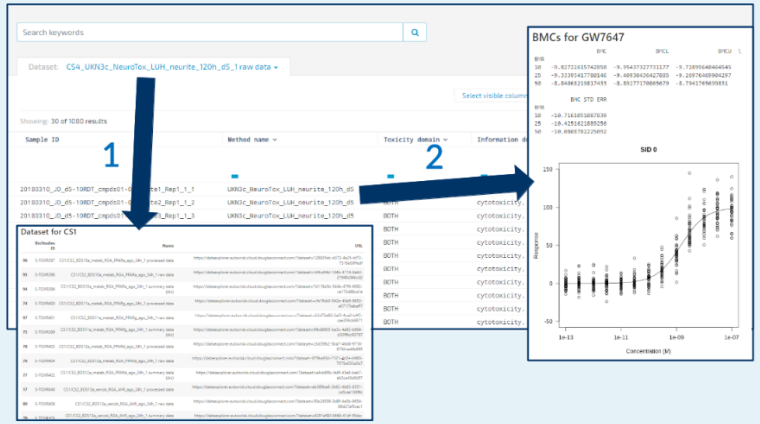
- A comprehensive tabular data and metadata environment
- Supports annotation, organisation and storage of primary data and metadata
- Provides domain data types (e.g. understand chemical's SMILES)
- Facilitates the analysis, visualisation and sharing of data
- Provides interactive exploration of the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



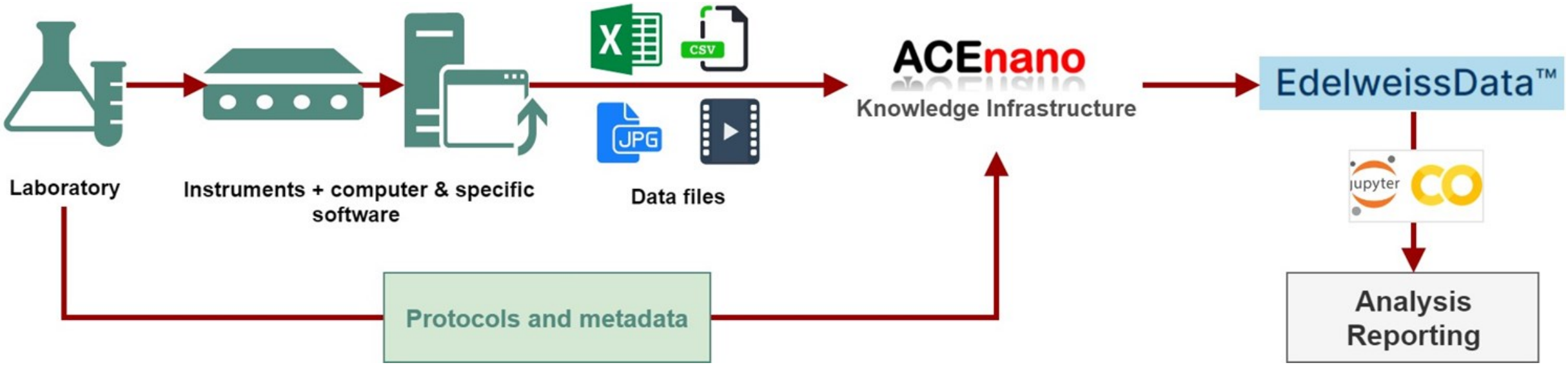




After indexing the data in EdelweissData, the APIs can be used to 1) show datasets from all partners relevant for a specific case study and 2) generate automatic workflows for further processing and analysis, e.g. the calculation of benchmark doses.



https://saferworldbydesign.com/edelweissdata/


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

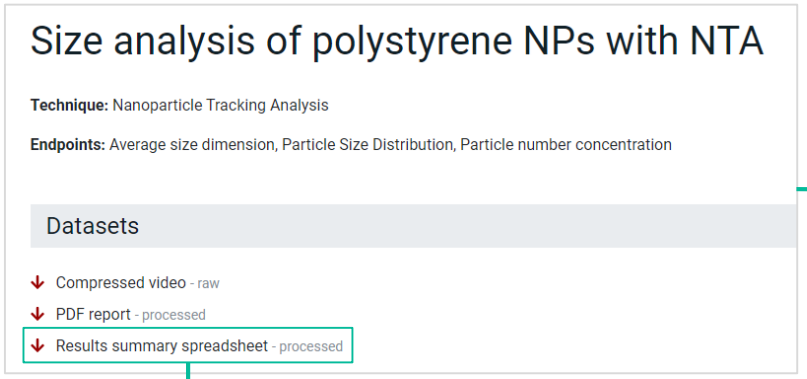
Use case: Nanoparticle Tracking Analysis (NTA)

Step 1. Addition of protocols

Step 2. Creation of data workflow

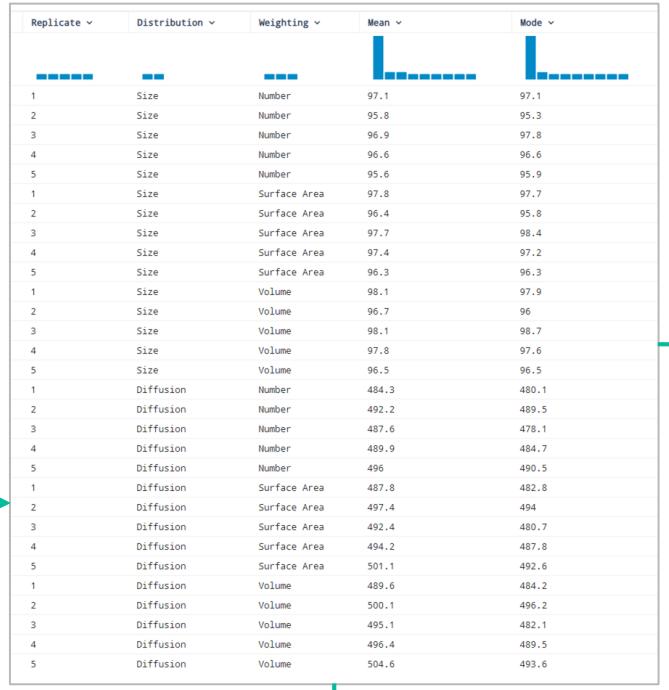
Step 3. Transfer of data to EdelweissData

- 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



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

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

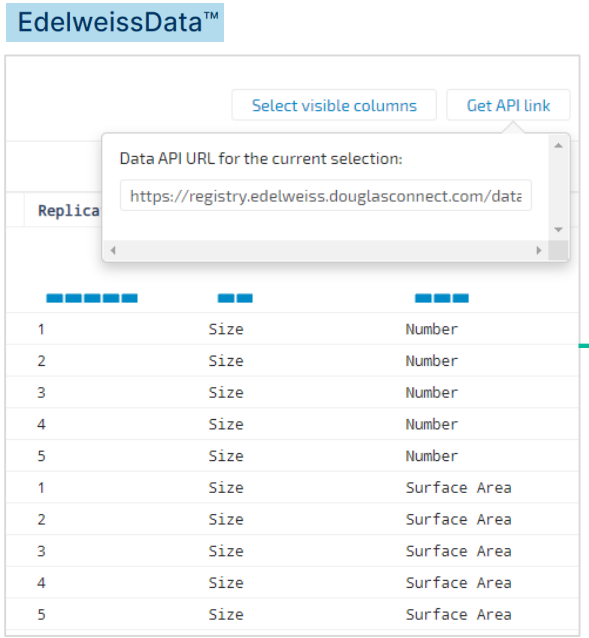
Step 4. Data analysis

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

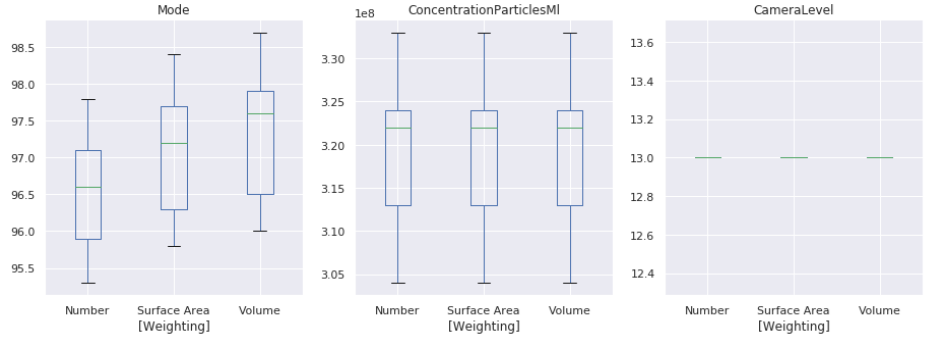
Use case: Nanoparticle Tracking Analysis (NTA)

Step 4. Data analysis

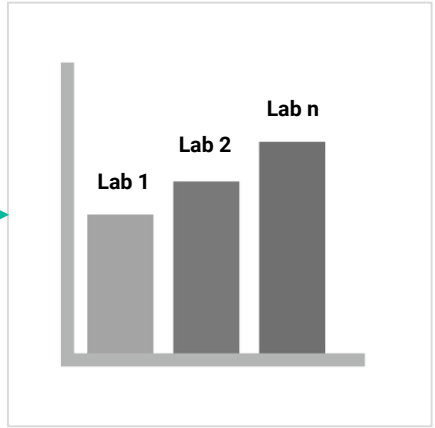
- Selection of dataset(s) to be analysed: data API
- Use the data API url (e.g. in JupyterLab or Google Colaboratory tools): extraction of relevant data, analysis, plotting, etc.
- Generation of a study report



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

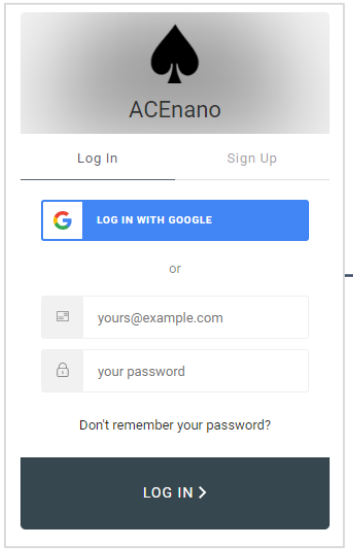
- User manual: https://github.com/NanoCommons/tutorials/tree/master/ACEnano manuals
- Poster summarising the KI's features: https://acenano.douglasconnect.com/dissemination/event/152/euronanoforum-2019/
- Contact and user support: acenano@edelweissconnect.com

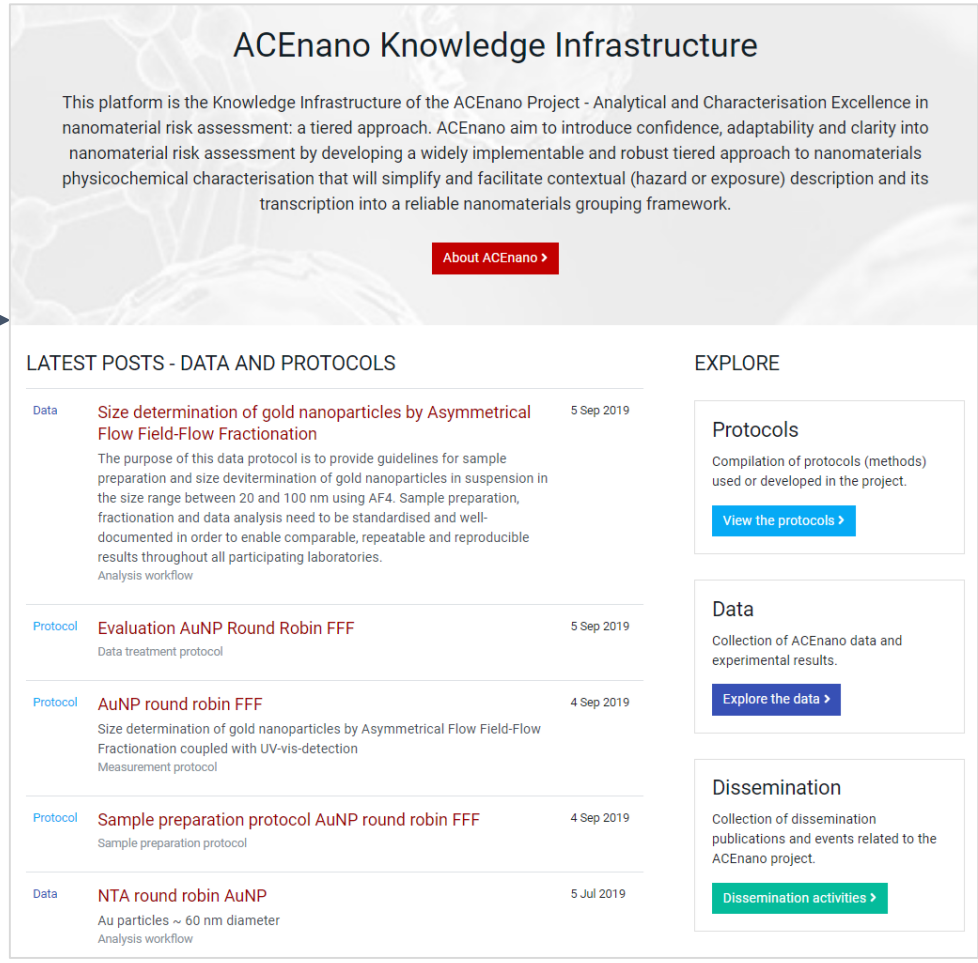
Next training session

- 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

Knowledge Warehouse





User manual:
https://github.com/NanoCommons/tutorials/tree/master/ACEnano 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

Google Drive content

11 NanoCommons Search for something... Go! Upgrade 391 Hi, Thomas Exner

Projects
Inventories
Protocols
Reports
Activities
Support
Settings
Academy

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.

Google Drive content

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

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

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:

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.).

Variant of this protocol:

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.

Protocols: sample preparation

Part 2: Steps

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

Step #: 1 **Action:** 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

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

Protocols: measurement

Part 3: Steps

Protocol steps

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

Step #:* **Name:***

0

Description:*

Image (optional)

Choose File No file chosen

Caption

delete

Delete this step

+ Add another step

Preview protocol

Submit protocol

Make more changes

Protocols

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.

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)

Linked to datasets

Discussions

Questions?

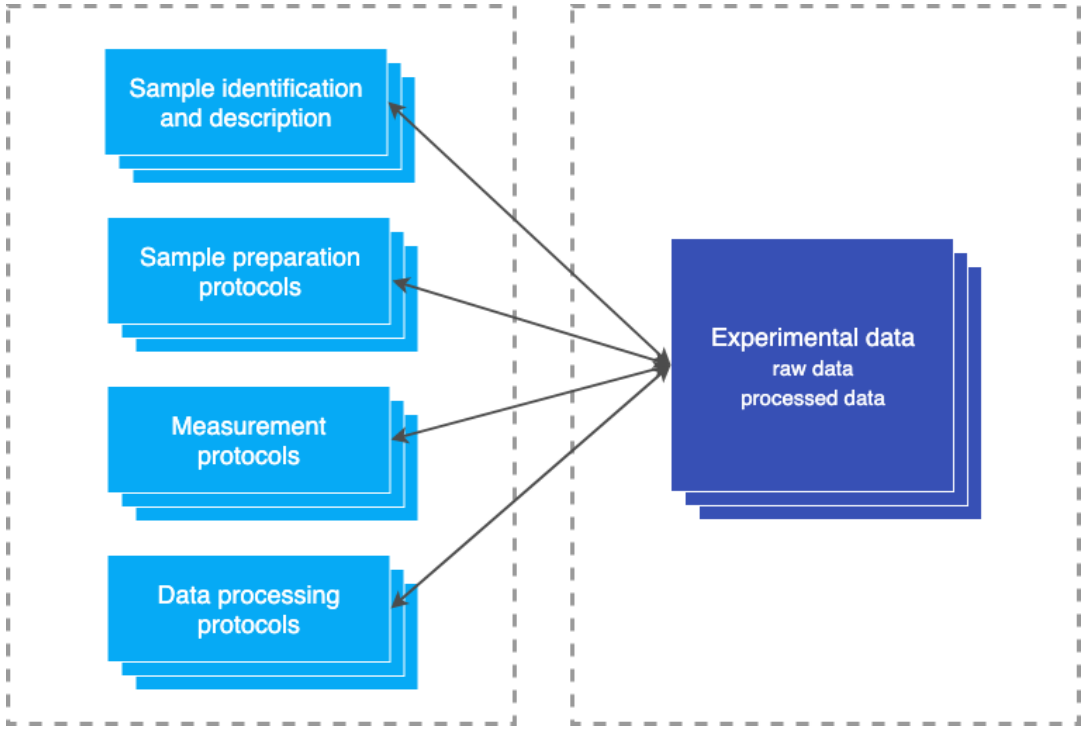
Give us feedback: https://it.research.net/r/calibrateusertesting

Hands-on session: Data

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.



Data workflow and data upload

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

Select a protocol for preview

3

Protocols

Select the measurement protocol used in your analysis.

Measurement protocol:

Continue to next step

Select a protocol for preview

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

Data workflow and data upload

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:

First name *

Last name *

Email *

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

Data workflow and data upload

7

Data files

Dataset type:* Raw | **Dataset name:*** | **Upload dataset:*** Choose File No file chosen

Delete this dataset

Dataset type:* Processed | **Dataset name:*** | **Upload dataset:*** Choose File No file chosen

Delete this dataset

+ Add dataset

Submit your data

Technique | Organisation | Filter | Reset

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

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

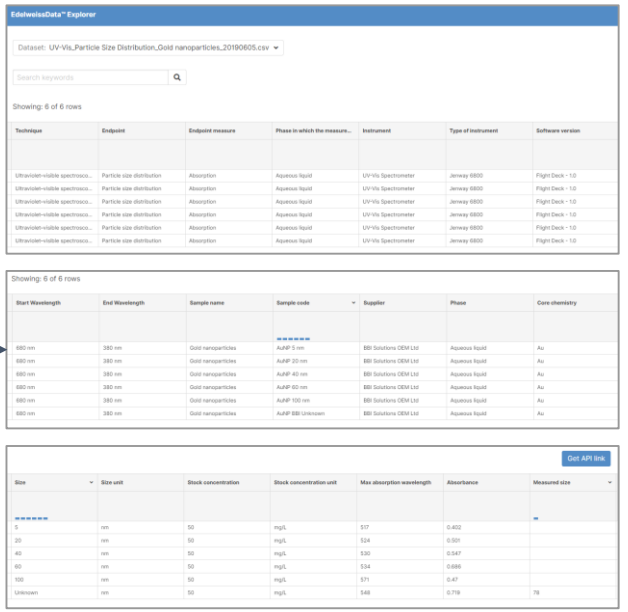
For technique: Ultraviolet–visible spectroscopy
For endpoints: Average size dimension, Particle Size Distribution

1 **Vortexing** Mixing and dispersing of nanoparticles that are suspended in a liquid phase

Speed:	/
Duration:	2 min
Phase change:	Aqueous liquid → Aqueous liquid

2 **Dilution** Additional dilution of original sample for analysis

Data - view, filter, analyse, API



EdelweissData™

Discussions and conclusions for the day

Questions?

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

ACEnano

Analytical and Characterisation Excellence

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

Thank you for your attention!

Introduction to the annotations / ontology topic

Short introduction to ontologies

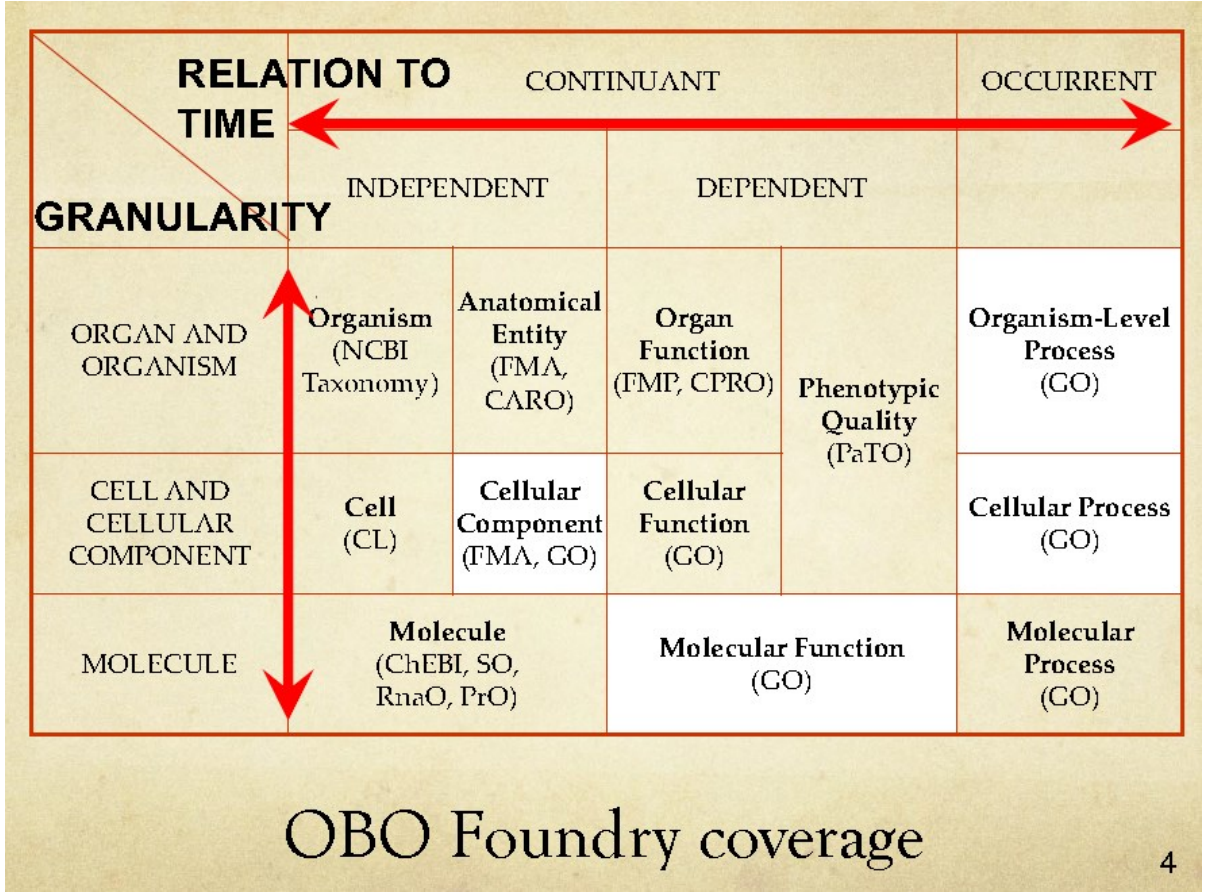
- Evolved from the interoperability requirement for system integration
  - data heterogeneity
  - semantic heterogeneity

- 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.

Short introduction to ontologies

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.



Provided by George Gkoutos, UoB

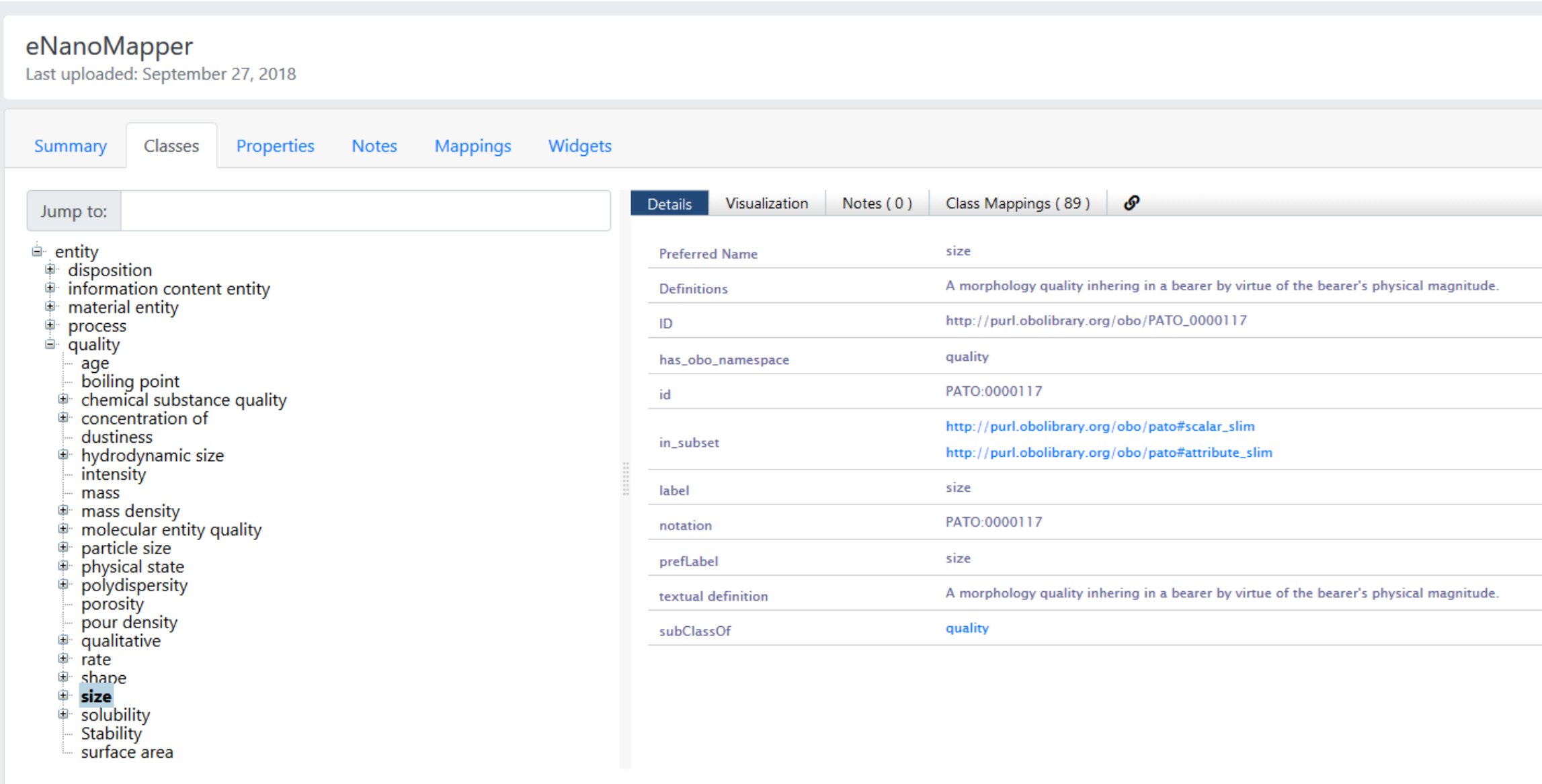
Short introduction to ontologies

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.

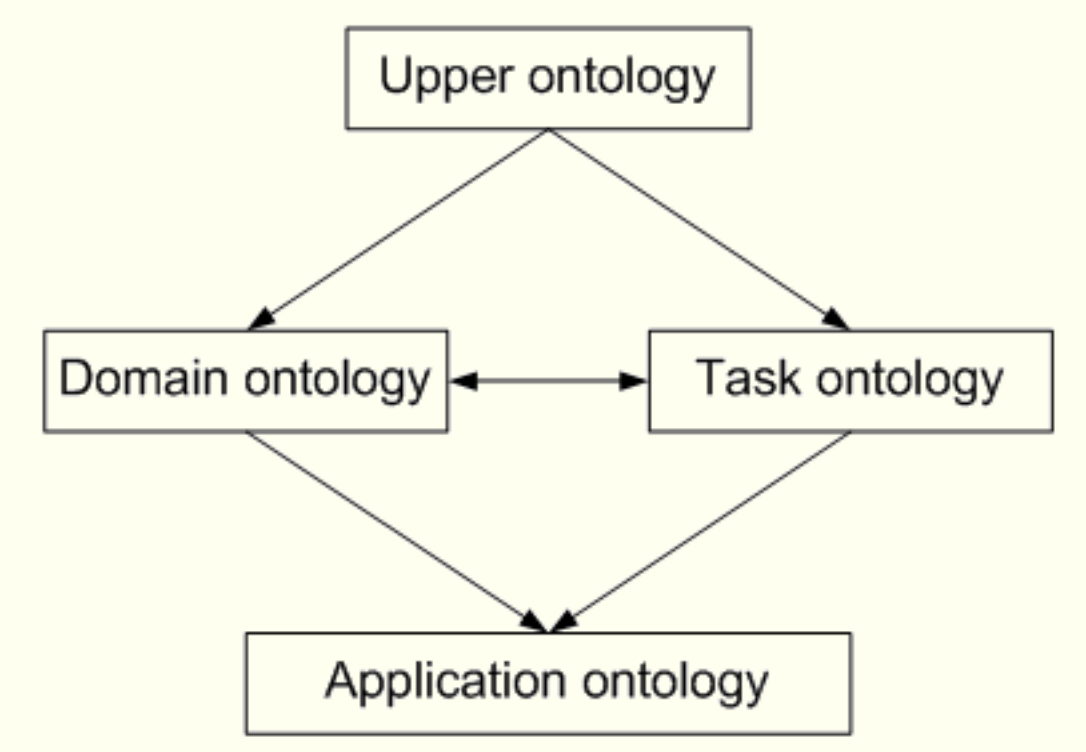
Short introduction to ontologies



Short introduction to ontologies

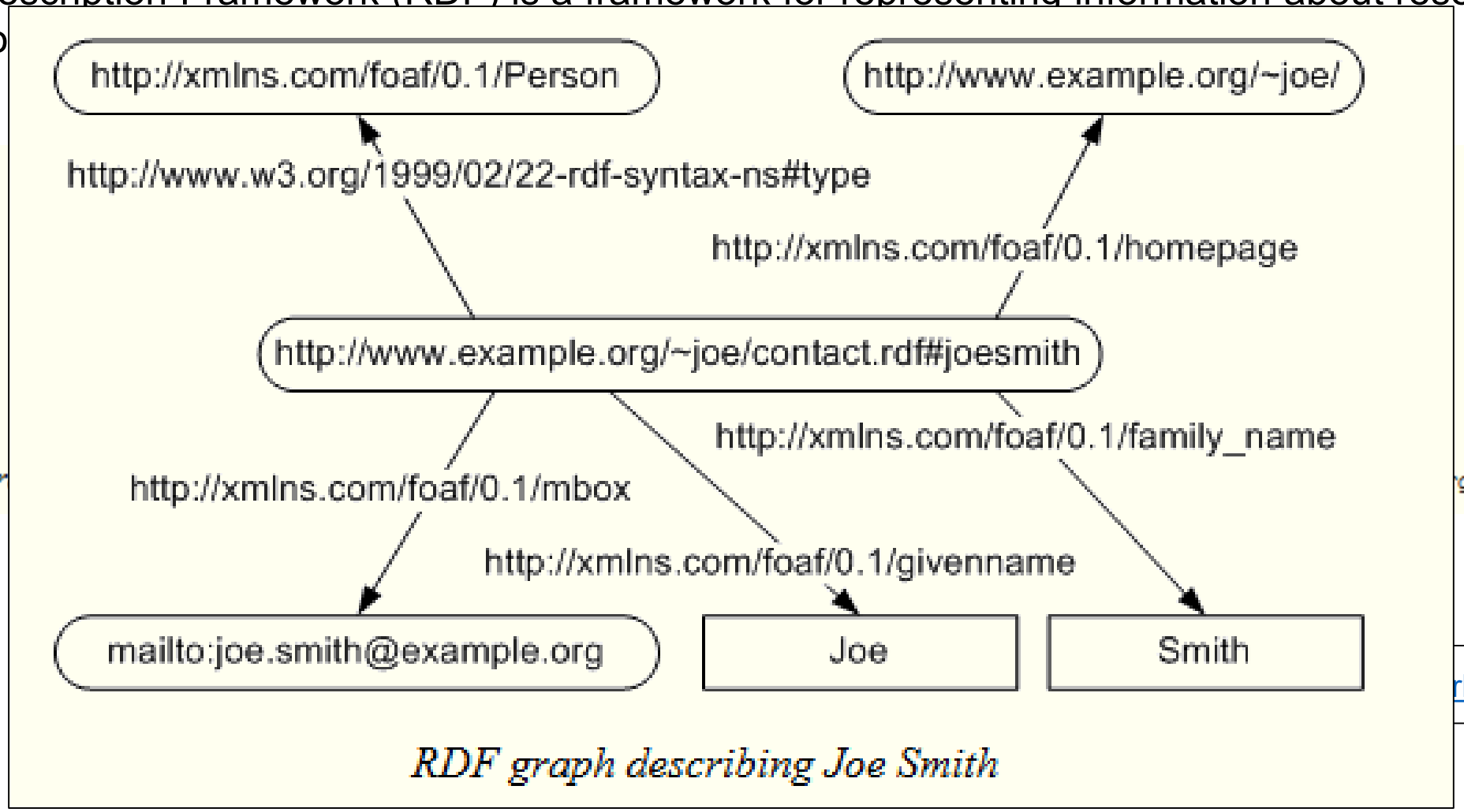
The modular design uses inheritance of ontologies

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



Resource Description Framework (RDF)

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



RDF graph describing Joe Smith

RDF triple (in gr

g/~joe/"

rk.html

Semantic annotation

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.

Endpoint: http://www.bioassayontology

VSSA: http://purl.enanomapper.org/onto/ENM_0000091

Technique: http://purl.bioontology.org/ontology/npo#NPO_1405

not available

Raw data: http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus

Parameters: http://ncicb.nci.nih.gov/xml/owl/EVS/Th 0474

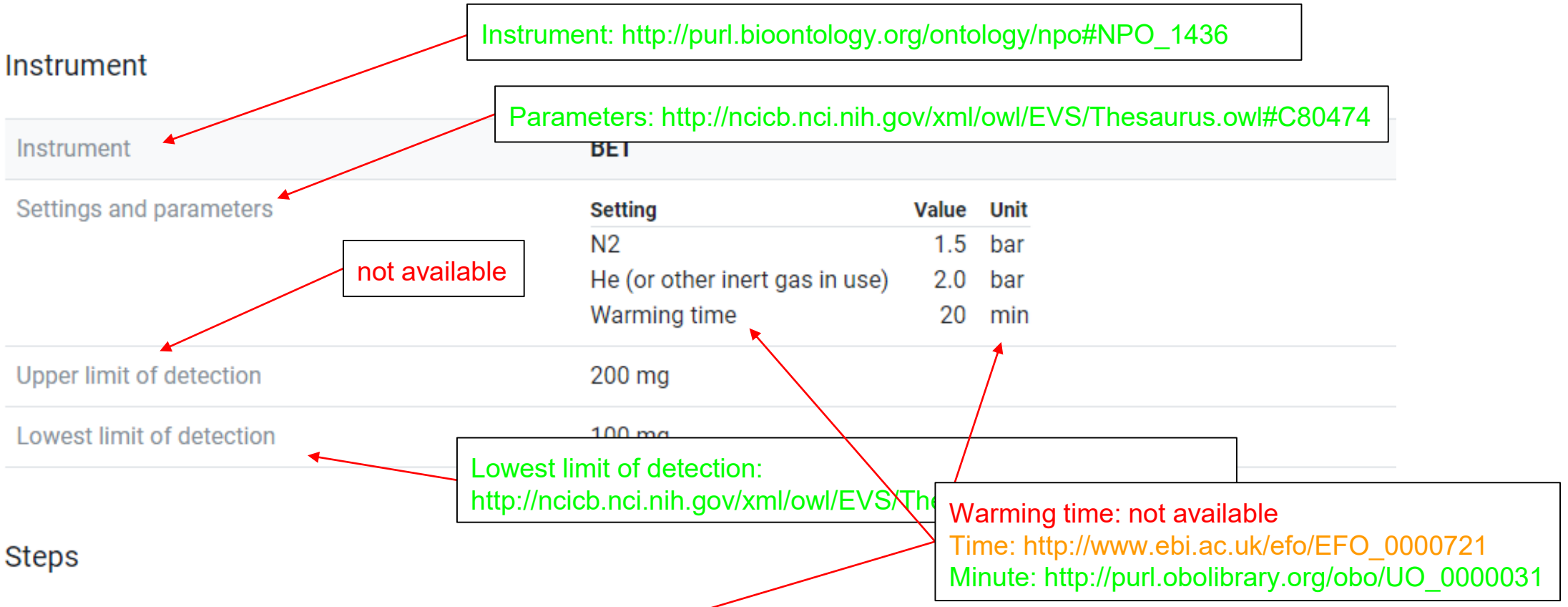
not available

Phase: http://purl.bioontology.org/o

Powder: http://purl.bioontology.org/ontology/npo#NPO_915

Measurement	
Endpoints	
Technique	
Type of raw data produced	– BET Specific Surface Area using 5 isotherm data points at the adsorption branch of the isotherm
Measurement quality parameters	– p/p0 last adsorption isotherm data point taken a first isotherm data point taken at p/po – *common setting:* 0.01- 0.05
Phase in which the measurement is performed	Powder

Semantic annotation



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	NA	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 bee reduced, **2. We only use dilution factor**
Drying	http://purl.bioontology.org/ontology/npo#NPO_1956	ENM	NA	Missing in BioPortal	The removal of water or solvent from a sample by evaporati
Vortexing	http://purl.bioontology.org/ontology/npo#NPO_1952	ENM	NA	Missing in BioPortal	The mixing of liquids to produce a more homogenous sampl 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	NA	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	NA	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/1mqt4epvvXMDFjipO5KeY_2u135WFXAhJfEXY4mkZH-A/edit

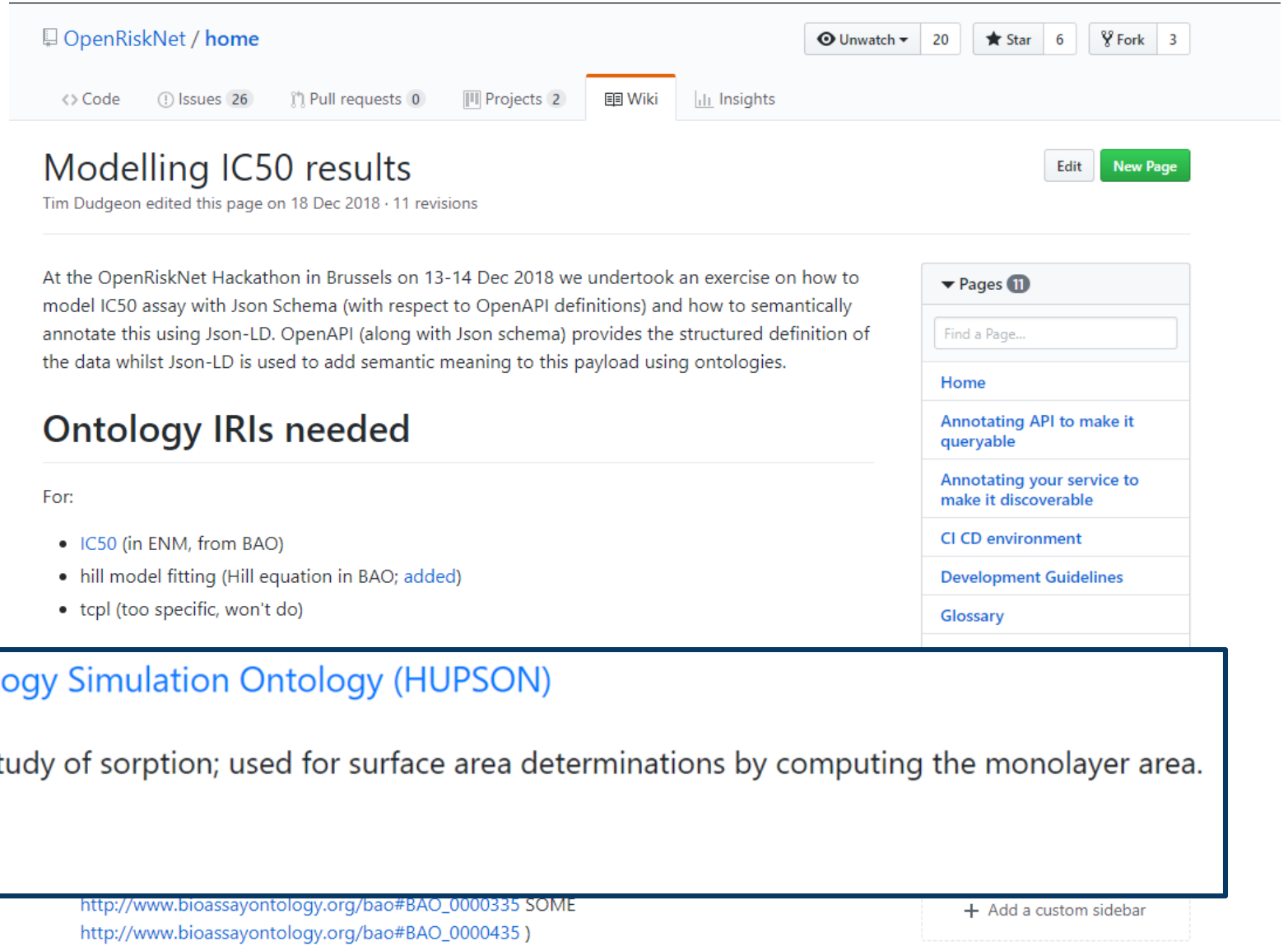
Complex classes

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

Edit New Page

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

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

+ Add a custom sidebar

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

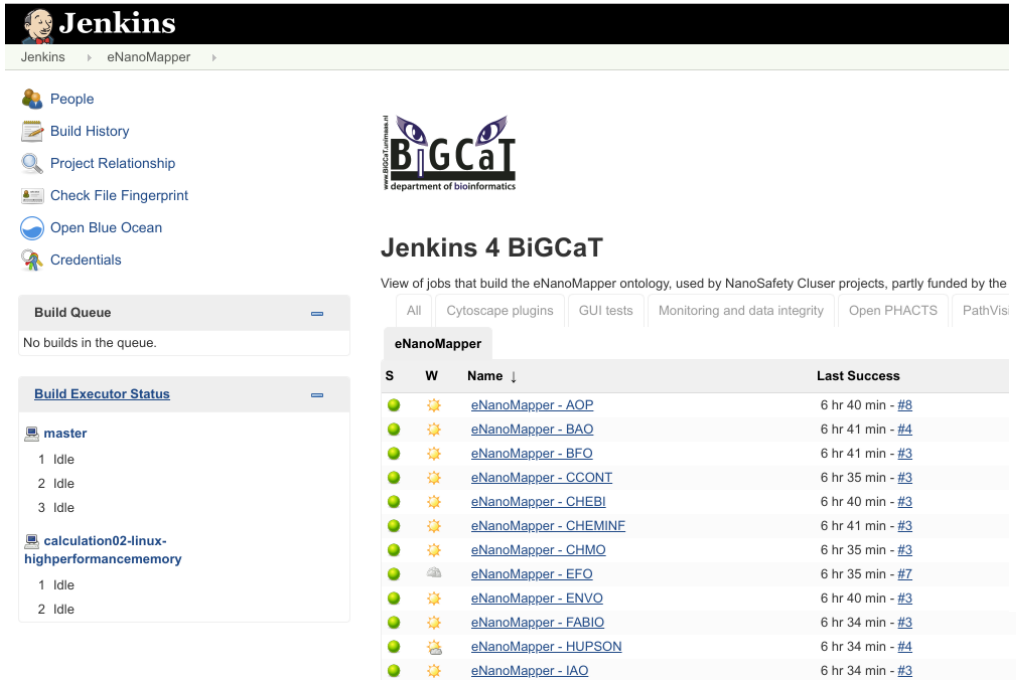
http://scai.fraunhofer.de/HuPSON#SCAIVPH_00000105

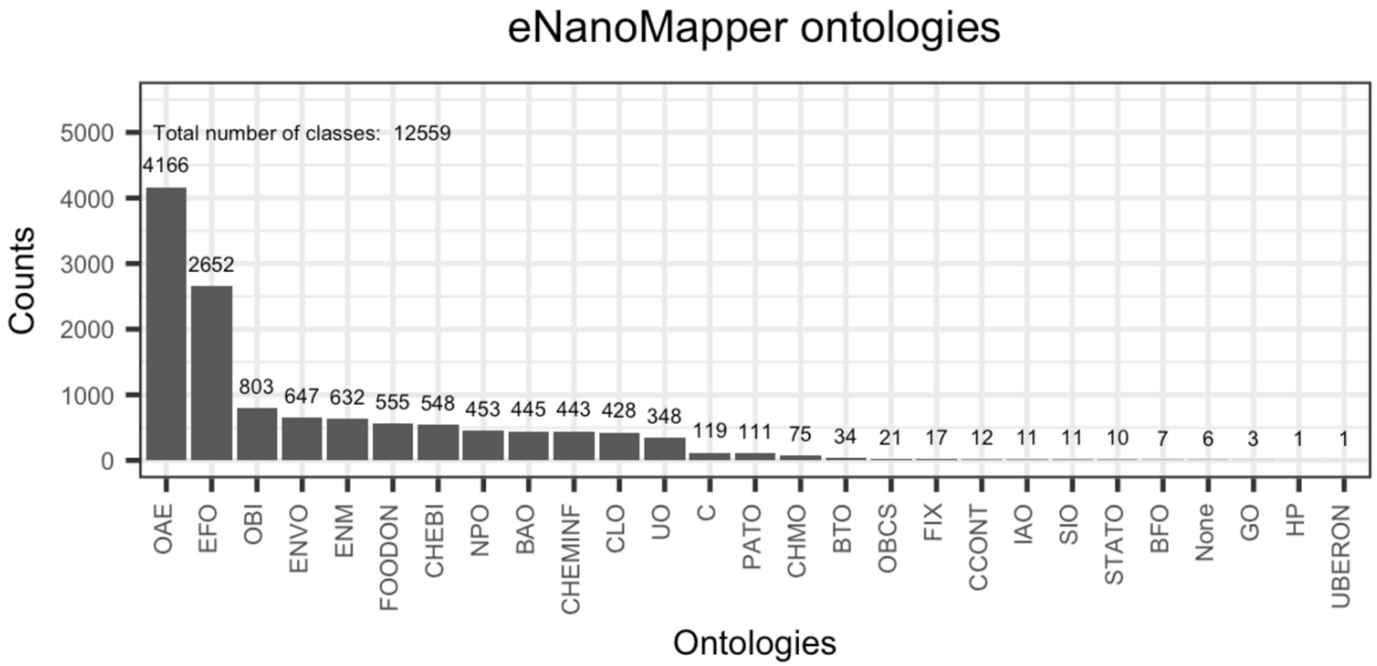
An extension of the Langmuir isotherm equation in the study of sorption; used for surface area determinations by computing the monolayer area. Abbreviated BET equation. source: ...

details - visualize

http://www.bioassayontology.org/bao#BAO_0000335 SOME
http://www.bioassayontology.org/bao#BAO_0000435)

eNanoMapper ontology





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: Is there anything out there?

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

Enter a class, e.g. Melanoma

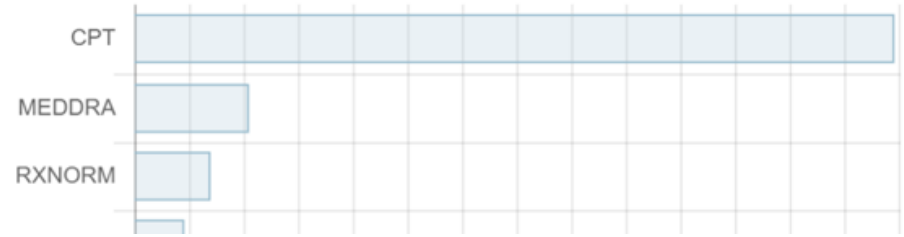
Advanced Search

Find an ontology

Start typing ontology name, then choose from list

Browse Ontologies

Ontology Visits (August 2019)



BioPortal Statistics

Ontologies	815
Classes	9,958,055
Resources Indexed	48

Annotation of protocol structure

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: 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 mm 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. Source: https://en.wikipedia.org/wiki/Transmission_electron_microscopy

BioPortal
NanoParticle Ontology

Details | Visualization | Notes (0) | Class Mappings (35)

Preferred Name	transmission electron microscopy
Synonyms	TEM technique
Definitions	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] <ncicp:ComplexDefinition><ncicp:def-definition>An electron microscopy technique based on the use of transmission electron microscope.</ncicp:def-definition></ncicp:ComplexDefinition>
ID	http://purl.bioontology.org/ontology/npo#NPO_1430
comment	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]
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

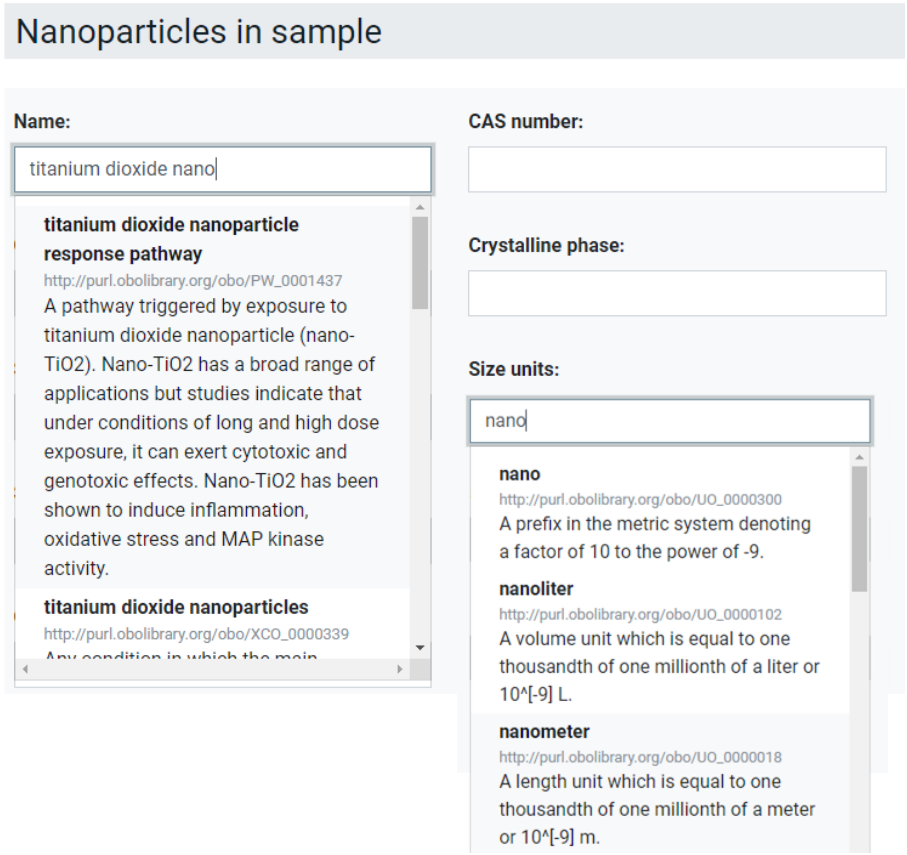
Name - Ontology URL:
Currently: http://purl.bioontology.org/ontology/npo#NPO_1699
Change: http://purl.bioontology.org/ontology/npo#NPO_1699

Details | Visualization | Notes (0) | Class Mappings (16)

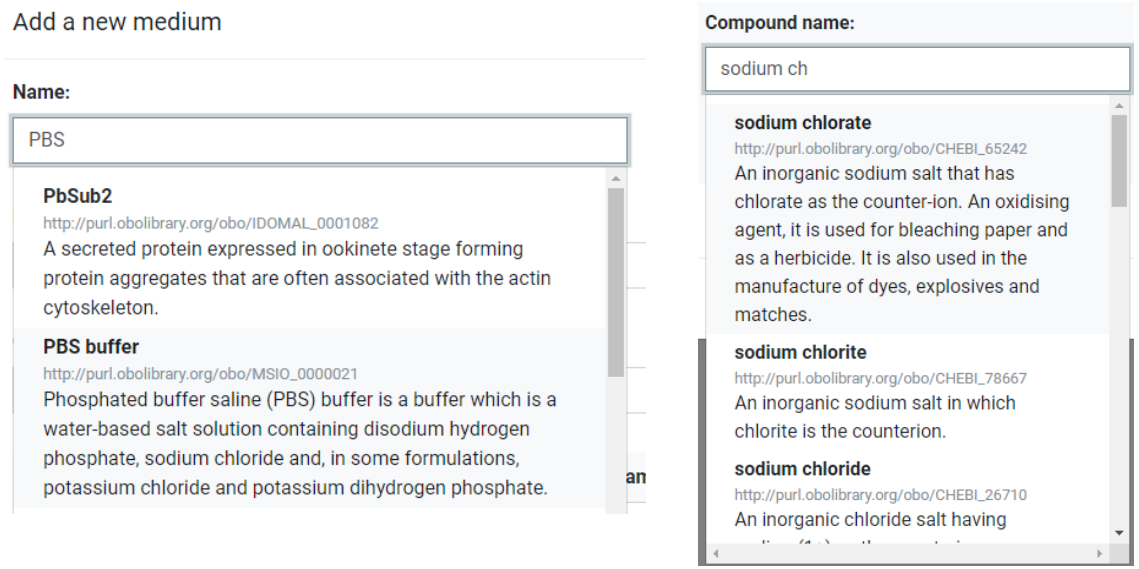
Preferred Name	particle size distribution
Definitions	<ncicp:ComplexDefinition xmlns:ncicp="http://ncicb.nci.nih.gov/xml/owl/EVS/ComplexProperties.xsd#"> <ncicp:def-definition>A size distribution inhering in particles.</ncicp:def-definition> <ncicp:Definition_Review_Date>100430</ncicp:Definition_Review_Date><ncicp:def-source>NPO</ncicp:def-source><ncicp:Definition_Reviewer_Name>Dennis Thomas</ncicp:Definition_Reviewer_Name> </ncicp:ComplexDefinition>
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

Ontology lookup service to support user input

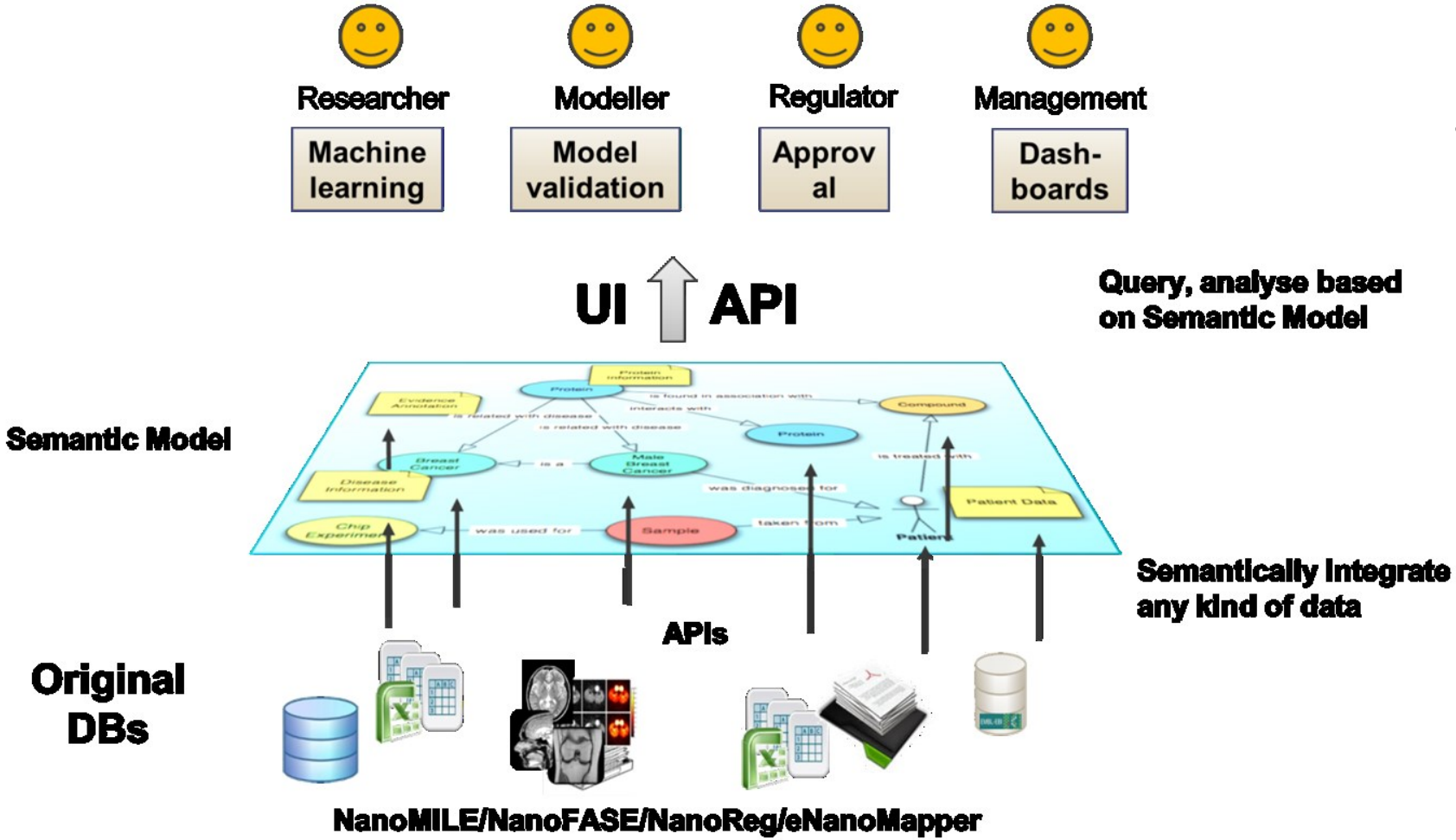
Description of Sample



Addition of media or compounds during sample preparation



Linking to other data sources



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

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Analytical and Characterisation Excellence

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Hands-on session: protocols and data annotations

Term collection:
https://docs.google.com/spreadsheets/d/1mqt4epvvXMDFjipO5KeY_2u135WFXAhJfEXY4mkZH-A/edit

BioPortal for searching ontologies:
https://bioportal.bioontology.org/

eNanoMapper ontology:
https://enanomapper.net/ontology and https://bioportal.bioontology.org/ontologies/ENM