



WP4 - Linking Ontology and Methodology

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Task 4.1 Ontologies



Sample Analysis BET UoB test

Measurement protocol

Endpoint: http://www.bioassayontology.org/bao#BAO_0000179

This protocol describes the measurement of the Brunauer, Emmett and Teller (BET) method.

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

Lawler, Emmett and Teller

Measurement

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

Endpoints

Volume Specific Surface Area (VSSA) / porosity

not available

Technique

Raw data: <http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C142663>

Type of raw data produced

- BET Specific Surface Area using 5 isotherm data points at the adsorption branch of the isotherm

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

- p/p0

Measurement quality parameters

Phase: http://purl.bioontology.org/ontology/npo#NPO_1610

last adsorption isotherm data point taken at p/p0 - common setting: 0.2

first isotherm data point taken at p/p0 - common setting: 0.05

Phase in which the measurement is performed

Powder

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



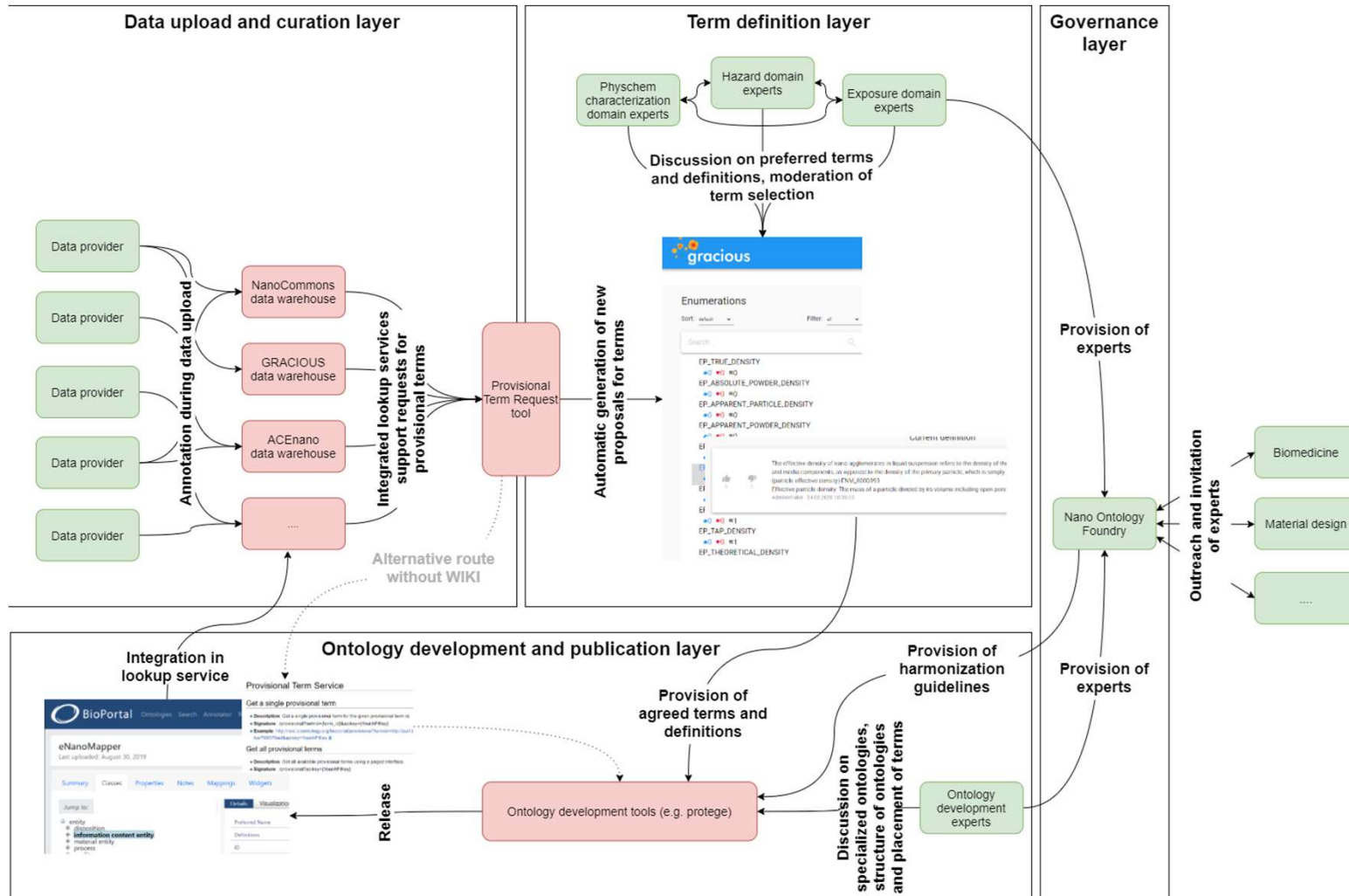
| Warehouse Term | Ontology URL | BioPortal Description | Comparison Descriptions | Specialists Description |
|---|---|---|-------------------------|--|
| Wide-Angle X-ray Scattering | http://purl.obolibrary.org/obo/CHMO_0000207 | A method for determining structure by measuring the change in direction 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 shear 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.enanmapper.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 been 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 |
| 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 high frequency to agi |
| 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 |

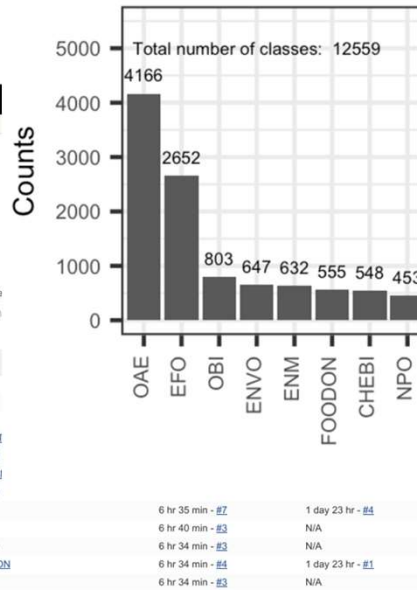
https://docs.google.com/spreadsheets/d/1mqt4epvvXMDFjipO5KeY_2u135WFXAhJfEXY4mkZH-A/edit



- Cooperation planned with NanoCommons and GRACIOUS
 - Defining the ontology universe
 - Organizing community-driven ontology development

- Provisional terms
 - Tool to request additional terms while annotating data
 - Ontology development team will be notified
 - Integration of tools in different ontology lookup services (Biomax, ACEnano)
 - Automatic update, when term is integrated in ontology





Section 1 of 6

NSC Ontology Task Force

The task force was created to generate a complete picture of the ongoing activities with respect to ontology development and data annotation within the projects of the NSC and other international groups.

Currently there are increasing needs of high quality data to feed into the evolving nanoinformatics workflows and for use in a regulatory and policy context. To achieve this, datasets need to be findable online and machine readable and able to be combined to larger datasets to be reused for the identification of hidden patterns and relationships as demonstrated, among others, by Labouta et al. (2019) during the meta-analysis of 93 peer-reviewed papers. Thus, datasets need to be annotated using established ontologies, along with communication between the various nanosafety databases/repositories. Currently, there is a number of parallel ongoing activities within the NSC projects for the development of data dictionaries (collections of terms), taxonomies and ontologies, which are focussed in a field-specific context. This potentially results in duplication of work and lack of communication between the various efforts, leading to lack of harmonisation and communication and to huge effort and time being wasted.

Aims of ac

- Generation of terms, taxonomies and ontologies.
- Identification on the similarities and alignment potential to promote a harmonised response of the nanosafety community and promote data interoperability and reusability, as per the requirements of the Open data initiative of the European Commission.

Even if the Task Force will end after the collection the above information, this should be followed up by the creation of expert groups. These groups will work on term collection in specific fields of nanosafety research

<https://forms.gle/EEgz5Vb36zcT2HrZ7>

| S | W | Name | Duration | Status |
|---|---|----------------------|------------------|------------------|
| ● | ● | eNanoMapper - AOP | | Success |
| ● | ● | eNanoMapper - BAO | | Success |
| ● | ● | eNanoMapper - BFO | | Success |
| ● | ● | eNanoMapper - CCONT | | Success |
| ● | ● | eNanoMapper - CHEBI | | Success |
| ● | ● | eNanoMapper - CHEBIJ | | Success |
| ● | ● | eNanoMapper - CHMO | | Success |
| ● | ● | eNanoMapper - EFO | 6 hr 35 min - #Z | 1 day 23 hr - #4 |
| ● | ● | eNanoMapper - ENVO | 6 hr 40 min - #3 | N/A |
| ● | ● | eNanoMapper - FABIO | 6 hr 34 min - #3 | N/A |
| ● | ● | eNanoMapper - HUPSON | 6 hr 34 min - #4 | 1 day 23 hr - #1 |
| ● | ● | eNanoMapper - IAO | 6 hr 34 min - #3 | N/A |


Releases after the management responsibility was transferred

- 5.0: 13 September 2018, 12,536 classes (update of CHEBI)
- 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 Terms)


Nano Safety Cluster Terminology

This Software is a system which aids agreement upon term definitions towards the creation of harmonized ontologies


Select a knowledge base to start



Nanoinformatics and simulations



Physicochemical characterization



Safe-by-design





Endpoint COPY ID

Enumerations

Sort: default Filter: all

Search

- Endpoint 2 0 3 cand. w.m.
- Physchem property endpoint 0 0 1 cand. w.m.
- Physchem characterization endpoint 0 0 1 cand. w.m.
- Action 0 1 2 candidate
- Action parameter 0 0 0 cand. w.m.
- Physchem characterization technique 0 0 0 cand. w.m.
- Brunauer–Emmett–Teller analysis 0 0 4 cand. w.m.
- X-Ray photon spectroscopy 0 0 0 cand. w.m.

Current definition

2 0

The endpoint is a quantitative or qualitative interpretable standardized representation of a perturbation (a change from a defined reference state of a "closed" model system) that is measured by the bioassay. An endpoint consists of a series of data points, one for each perturbing agent (screened entity) tested the assay. definition [http://www.bioassayontology.org/bao#BAO_0000179]
Thomas Exner - 17.09.2020 11:09:19

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Add new comment

ACEnano needs a very general definition for the data warehouse to cover all measured endpoints of the developed techniques. However, the expert feedback shows that very different definitions are possible and we might think of introducing another layer in the data warehouse to be able to annotate the data according to these different definitions with ontology terms for more specific endpoints (e.g. physchem property endpoint) and then also specifically search for them.
Thomas Exner - 17.09.2020 11:09:12

Proposal for ACEnano: The conclusion of a chemical reaction or a defined target outcome of an experiment; 2. An endpoint is the final stage of a period or process, i.e. in terms of ecotox testing such as reproduction success, mortality, growth or growth inhibition.
Thomas Exner - 17.09.2020 11:09:21

More specific endpoints, like physchem property endpoint, are used in eNanoMapper. Should this be added as an additional layer between result and the specific endpoints
Thomas Exner - 17.09.2020 11:09:11



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

Thank you for your attention!