NanoCommons

Nano-Knowledge Community

The European Nanotechnology Community Informatics Platform: Bridging data and disciplinary gaps for industry and regulators

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Summary

This deliverable describes the outcomes of the first 18 months of work on the NanoCommons Ontology, which builds on and expands the FP7-funded eNanoMapper ontology. With significantly fewer resources dedicated to ontologies than the eNanoMapper project had, the NanoCommons project has taken over the continued development of the eNanoMapper ontology, and the managed release of updated versions at regular intervals. NanoCommons has made two major releases of the ontology in a period of 18 months, based on needs from other NanoSafety Cluster projects and efforts, like Nanoreg2, Gracious, ACENano, the USA NIKC project, and the Malta Initiative.

This deliverable introduces the history of the eNanoMapper ontology, how the NanoCommons project has taken over release management, the recent updates to the development of the ontology and updates to the content of the ontology. It also describes our efforts for continued dissemination of the ontology to support others in utilisation of the ontology to support interlinking of datasets from different projects and sources and the collaboration with other projects with specific ontology work packages or tasks to guarantee a harmonized approach. Significant work went into maintenance of the ontology, requiring updates in third-party ontologies, updating the hosting of the ontology, and exploration of current needs from other European, American and international projects, and the integration of an ontology mapping tool for integration of datasets into the NanoCommons Knowledgebase. This deliverable also summarizes new dissemination and networking activities, consisting of both physical meetings and online tutorials, and an outlook of the upcoming work resulting from gaps identified in the reported initial ontology, which includes the need to add definitions to many of the terms, and to adjust the organisation of some of the terms based on user feedback.

Introduction

NanoCommons continues the NanoSafety Cluster ontology initiated by the eNanoMapper project. While there has been some discussion on whether the name of the ontology is suitable and encompassing, and various arguments have been made in favour and against a rename of the ontology, the name has not changed yet. On the one hand, it would be nice to have the name reflect either the current projects involved in it (like NanoCommons) or the NanoSafety Cluster, However, on the other hand, the current name has strong branding. For the time being, an intermediate solution has been found in clearly listing NanoCommons as being responsible for the current release management in the README as well as in the ontology metadata.

This deliverable describes the NanoCommons activities around the eNanoMapper ontology. It describes how the project took over the release management, how the ontology development system was managed, and how interaction took place with the EU NanoSafety Cluster community, and presents some future plans.

Ontology Development

NanoCommons took over the development of the eNanoMapper ontology (1–5) in January 2018 upon start of the NanoCommons project. This section describes the ontology source code, the automated ontology building tools, and updates on how the ontology is “hosted”, allowing it to be easily opened in tools like Protégé (6,7).

Ontology Source Code

The ontology continues to be developed on GitHub (https://github.com/enanomapper/ontologies). This allows the community development approach, which includes the ability to issue requests in the Issue Tracker, as several NanoSafety Cluster projects have done. Furthermore, the version control and text file basis of the ontology allows reviewing and commenting on changes, possibly following a “pull request” approach, which allows a formal review process (see details here).

Automated building

Maastricht University operated a Jenkins-based build server for the eNanoMapper ontology. The automated process allowed building of the ontology as soon as changes were made to the ontology. The latest version of the ontology was made available as a separate development version of the ontology. Because the same partner is also a partner in NanoCommons (the BiGCaT research group), the same system continued to be used. However, a security issue required the original Jenkins server to be taken down.

Over the period of July/August 2019 the ontology building jobs were therefore migrated to the Jenkins server of the BiGCaT department (https://jenkins.bigcat.unimaas.nl/view/eNanoMapper/). In this process, a security audit took place and the jobs were checked for possible security issues. The temporary unavailability of the build server also had the effect that the development version of the eNanoMapper ontology was unavailable in this period, as explained in the next section. Figure 1 shows the ontology "corner" of the BiGCaT Jenkins build server.

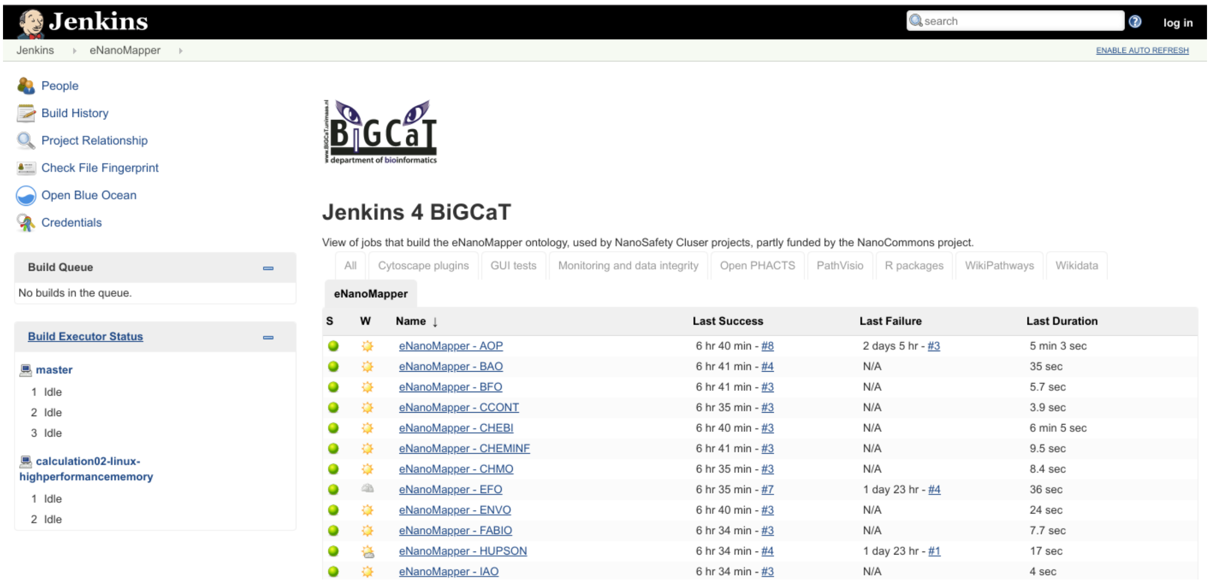

Figure 1. Screenshot of the eNanoMapper ontology building jobs on the Jenkins build server.

As part of the building, the testing of the ontology has also been migrated to the new Jenkins server. The original http://jenm.bigcat.maastrichtuniversity.nl link now redirects to the new server.

Finally, as part of this migration, we were required to update the Slimmer tool to the latest version of OWLAPI (8), version 5.1.11. This involved a few API changes, prominently a move from Java iterators to the `Stream` approach. This also highlighted two bugs in upstream ontologies, CHEMINF and BAO, which both suffered from circular dependencies (where two components of the ontology depend on each other). For the CHEMINF ontology this was fixed, and for BAO an issue report was filed and the problem was temporarily worked around using a merged ontology provided by the BAO project itself.

Ontology hosting

The eNanoMapper ontology was previously hosted by the eNanoMapper project. This allowed the setting up a *purl.enanomapper.net* domain from which the various Web Ontology Language (OWL) files could be served. This domain was used for both the released and the development version of the ontology. The advantage of this was that the OWL files could be located at different locations. For example, the development version of various OWL files were hosted by the aforementioned Jenkins build server. However, during the first 18 months of the project the purl.enanomapper.net domain stopped working as a consequence of the limited possibilities to maintain the infrastructure after the end of the eNanoMapper project and different, better sustainable approach was adopted.

The choice was made to host the OWL files from GitHub instead for the released version of the ontology, and have the development OWL point directly to the Jenkins build server. The GitHub hosting of OWL files was formalized in the 5.0.2 release (27 July 2019), and the development OWL file (http://enanomapper.github.io/ontologies/enanomapper-dev.owl) point to the new Jenkins build server was implemented in the 6.0 release. Guidance and documentation have been updated to refer to the new ontology URLs.

The release process has, however, not changed. When a stable release is made, the slimmed ontologies are copied into the GitHub source repository and become available to the released OWL as before.

The Ontology

No significant changes were needed to fulfil the extended requirements from the NanoCommons project until now, but the ontology has undergone maintenance and seen extensions to fit the current, active uses of the ontology mainly in the running projects of the EU NanoSafety Cluster. This section discusses the changes made in the first 18 months of NanoCommons.

Third party ontologies used

The list of third-party ontologies that the eNanoMapper uses has slightly grown (see Figure 2). Because the ontology is built from slimmed down versions of those third-party ontologies, they all get automatically updated to their latest version. That said, some bigger changes happen that affect the NanoCommons ontology. Some examples of these changes are listed below.

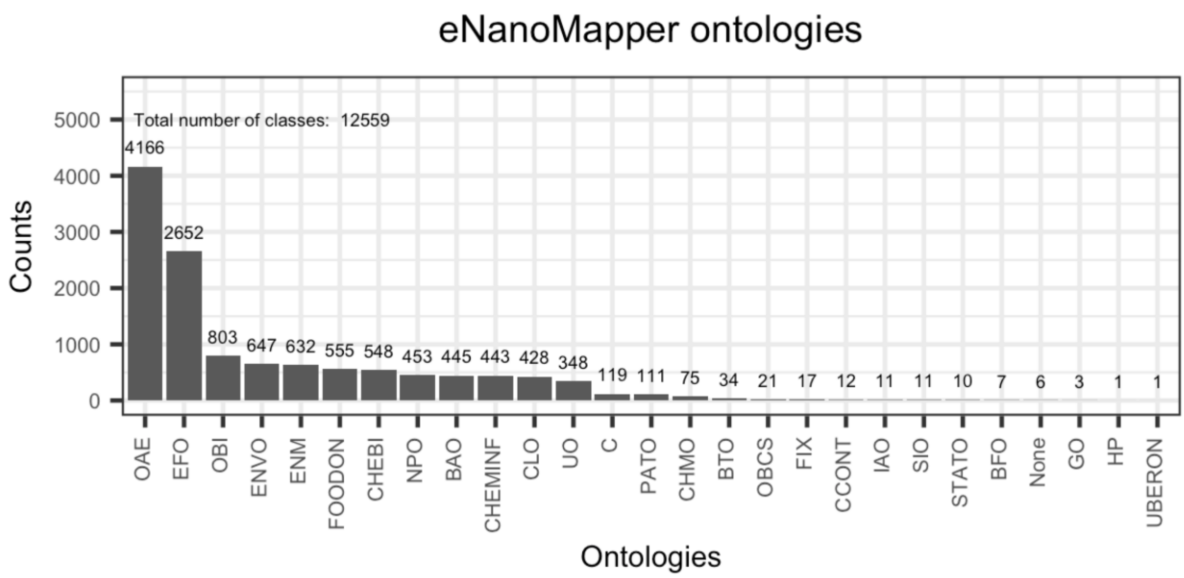

Figure 2. Ontologies of which slices are imported with the Slimmer tool into the eNanoMapper ontology (version 5.0.2).

First, the Basic Formal Ontology (BFO) (9) released their version 2 ontology, and other ontologies started updating to this release. The Semanticscience Integrated Ontology (SIO) (10) and CHEMINF ontology (11) got updated. The update of the latter resulted in inconsistencies in the eNanoMapper ontology, which the Maastricht University team addressed by first updating the CHEMINF ontology to be based on BFO 2. This development took place in the GitHub repository of CHEMINF, where it migrated after the Google Code closed down[1]. After this issue was resolved, the eNanoMapper ontology was updated accordingly.

The 5.0 release of the eNanoMapper ontology also added two new upstream ontologies, FRBR-aligned Bibliographic Ontology (FABIO) (12) for bibliography-related terms and the Adverse Outcome Pathway (AOP) ontology (13). Release 6.0 added for the first time terms from Wikidata (14) as an OWL file, for the OECD testing guidelines (see below). Formally, however, Wikidata is not an ontology.

Ontology Releases

The first major release under the supervision and management of NanoCommons was the 5.0 release (https://github.com/enanomapper/ontologies/releases/tag/v5.0), made on September 13 2018, nine months after the start of the project. This release included the updated CHEMINF ontology (see previous section) and a number of new terms, following needs identified from collaboration projects. The major release was followed by a minor release (5.0.1) on 27 September 2018, both of which have been distributed via BioPortal (http://bioportal.bioontology.org/ontologies/ENM). This release had 12,536 new terms. It was followed by a 5.0.2 release, fixing a loading issue, but that was otherwise identical to 5.0.1 (see the *Ontology hosting* section). The 2018 release generated quite significant traffic and interest, as shown in Appendix 1.

The second major release was the 6.0 release (https://doi.org/10.5281/zenodo.3382100), made on August 30 2019. This release again added a number of terms used by other projects, among which the OECD Testing Guidelines (see Figure 3, and the next section). This release had 12,732 new terms.

[1] https://github.com/semanticchemistry/semanticchemistry.

Collaboration and harmonization with other nano ontology development efforts

Ontology Terms for the OECD Testing Guidelines

One of the purposes to have an ontology is to be able to identify things. To support the *Malta Initiative* (https://www.nanosafetycluster.eu/international-cooperation/the-malta-initiative.html), terms for 32 OECD Testing Guidelines have been added to the ontology, as shown in Figure 3. It was chosen to use Wikidata and Scholia (15) for this, providing a graphical, interactive interface to explore the testing guidelines (see Figure 4).

Figure 2. Screenshot of Protégé showing the *guideline* concept added in release 6.0 of the ontology, along with various OECD Testing Guidelines.

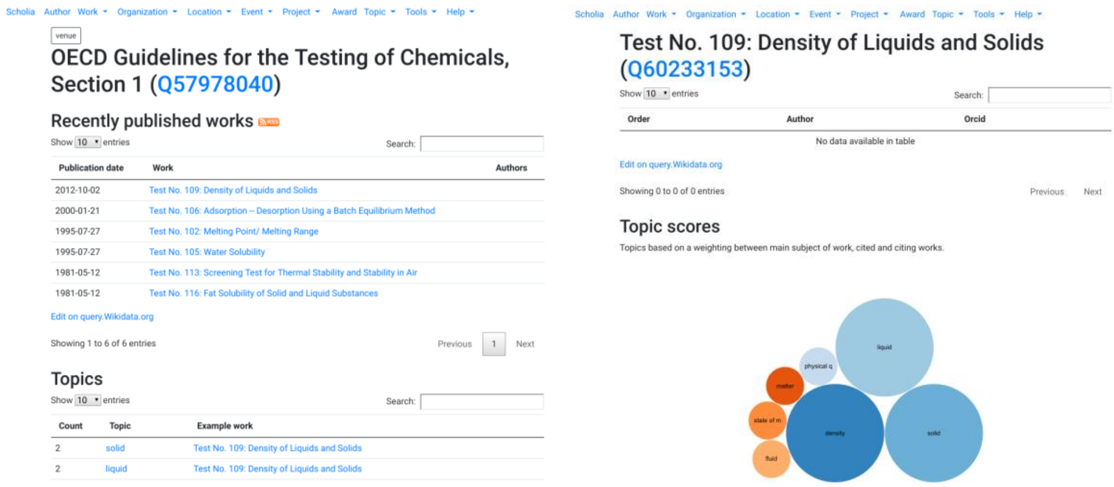

Figure 4. Screenshots of Scholia showing Section 1 of the OECD Guidelines for the Testing of Chemicals (left) and part of what Scholia shows for the OECD guideline, "Test No. 109: Density of Liquids and Solids" (right).

Alignment with the NanoInformatics Knowledge Commons (NIKC)

The NIKC (http://nikc.egr.duke.edu/) is an infrastructure developed by the NanoCommons partner the Center for the Environmental Implications of Nanotechnology of Duke University, U.S.A. NIKC consists of a data repository and associated analytical tools, which were developed to work with the integrated datasets. NIKC consists of already published peer-reviewed data and metadata on the intrinsic, extrinsic and social properties (e.g. anticipated use scenarios, matrix, concentration in products) of NMs, the characteristics of the environment in which the NMs are exposed, and relevant exposure and hazard measurements.

The NIKC structure can accept data of varying granularity levels, in terms of experimental complexity and richness. It was recently modified to be able to accept raw and calculated experimental data captured during simple and complex experimental processes. NanoCommons partners Biomax is implementing a European version of the NIKC, which is slightly modified from its U.S. counterpart in order to meet the needs of EU funded projects and to comply with the EU's legal framework. The two different NIKC mirrors will be perfectly compatible and will be able to exchange data based on the licenses of the specific datasets uploaded into either version.

To achieve all this, the NIKC structure has been built with consideration of existing ontologies and controlled scientific vocabularies within the nanotechnology and nanosafety fields. NIKC developed the nano-dictionary, a dynamic taxonomy that contains the terms used in the data repository and is continuously being expanded as more data are curated. The nano-dictionary, initially drew terms from the eNanoMapper ontology, and where terms could not be identified from existing ontologies and other sources (e.g. scientific vocabularies, peer-reviewed publications) these terms were defined through the collaboration of the curating team with relevant experts (e.g. toxicologists, materials scientists). The need for harmonisation and data interoperability led to close collaboration between the NIKC team with NanoFASE and NanoCommon teams. Due to NanoCommons being the leading party in semantic annotation, the NIKC team started harmonising the data-dictionary further with the eNanoMapper ontology. To increase the interoperability between the two, a close collaboration between the NIKC curation team and NanoCommons partners Maastricht University, one of the responsible partners for developing the NanoCommons ontology, is ongoing. Through these interactions, terms in the nano-dictionary that are missing in eNanoMapper are being defined and added to the relevant ontological branches, and semantic mapping is being established between the two vocabularies. The 2nd NanoCommons release, eNanoMapper 5.0.2 contained 12,559 terms from 27 different ontologies (see Appendix 1). The NIKC dictionary contains 470 terms. Out of these 470 terms, a total of 114 terms of the NIKC dictionaries are already present in the eNanoMapper ontology; 144 terms are not present but belong to ontologies that are part of the eNanoMapper ontology; and 212 terms are not present and are part of external ontologies. The latter two categories are in the pipeline to be added to the eNanoMapper ontology after expert review. Additionally, the collaboration will be continued for the entire project duration and is envisaged that in the mid-term the two approaches will be fully aligned and any further additions will be automatically added in both the eNanoMapper/NanoCommons ontology and the NIKC nano-dictionary.

ACEnano protocol annotation

H2020 project ACEnano (www.acenano-project.eu) aims 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. To enhance standardization of approaches and track the influence of utilisation of harmonised approaches as slight modifications of these on the results obtained from new methods and achieve reproducibility across different laboratories of more established methods, metadata detailing the experimental setup has to be stored as part of the protocols and preferably also be differently associated with the data. The questionnaire-like protocol reporting tool developed in ACEnano collects such metadata by guiding the user from the initial steps (e.g. sample description, sample preparation) to the actual measurement relevant to different endpoints and appropriate techniques for physico-chemical characterisation, through to the data processing steps.

To integrate this unique protocols database approach within the NanoCommons knowledge infrastructure and make it interoperable with other data sources, annotation of the protocol description and the (meta)data model are underway, supported by NanoCommons. The protocol interface and existing protocols uploaded to the repository were screened for specific terms or groups of terms, which should be stored in a semantically annotated form as part of the protocols and metadata of datasets. The focus for a first round of annotation was put on the terms that are essential for the identification of relevant protocols (experimental method, nanomaterial pre-characterization to select appropriate methods, etc.) and to compare different variants of the protocols on a high level (e.g., effect of different sample preparation steps influencing the results, etc.). Manual search for these terms showed that annotation of starting materials is possible to a large extent with terms available in the eNanoMapper ontology, while experimental setups and parameters needed to include terms from other ontologies or are not covered at all at the moment. The generated list of required new ontology terms (see Appendix 2) is now being evaluated by NanoCommons ontology experts and prepared for integration into the next NanoCommons release of the eNanoMapper ontology. This will use the concept developed in the ontology hackathons (see below) to construct complex terms from simpler ones with the advantage that the hierarchies of the underlying simpler terms can be used to help place the object in relationship to other objects of the protocol or in the protocol repository.

Tools development for annotation

A first version of the NanoCommons tool for ontology-based annotation was deployed via the NanoCommons portal during the 1st ontology Hackathon, October 2018 in Athens. The work process presented and evaluated by the Hackathon participants was based on two steps, an upload of the definitions of the measured parameters (the metadata) and the actual data upload. The definition of the measured parameters is based on assignment of ontology terms. Ideally a single specific term is already available from a given ontology. For example to define a parameter “DLS” the ontology term “NPO_1469 dynamic light scattering” provides a full definition (see Figure 5).

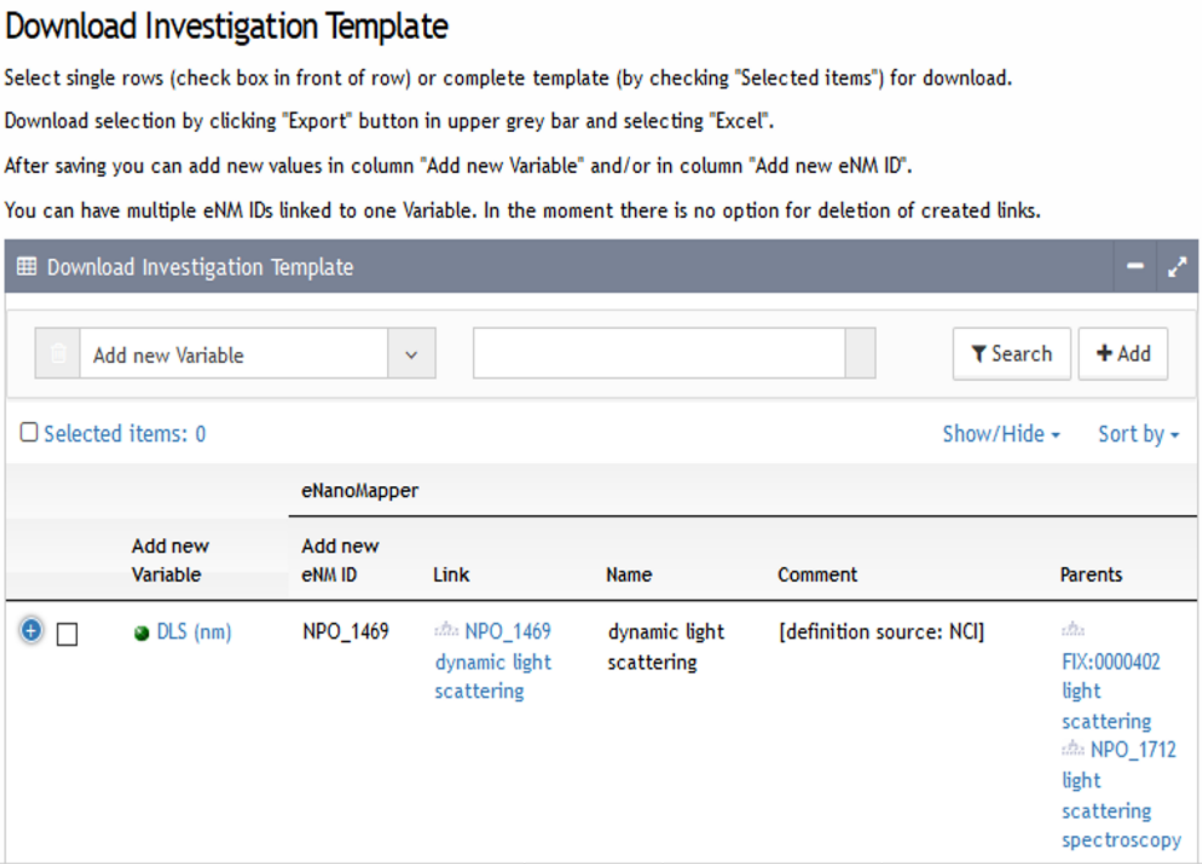

Figure 5. Definition of the parameter “DSL” during the 1st NanoCommons Hackathon by assigning an ontology term. NPO_1469.

However, for parameters not yet included into any ontology a "post-coordination" approach is used. In this approach the users decide to combine several existing ontology terms which, in combination, provide the definition of the measured parameter. To aid this approach a cross-ontology search and browse tool was provided in the NanoCommons portal which suggests matching ontology terms for user provided keywords (Figure 6). The advantage of post-coordination compared to the standard pre-coordination approaches are the much smaller number of required terms and the ability to express meaning that has not yet been ontologically encoded. The disadvantage is that consistency of post-coordination use of terms between different users is hard to ensure. Therefore, we plan to extend the current NanoCommons portal to include a similarity searches of uploaded parameter definitions to already existing definitions to avoid redundant but slightly different parameter definitions.

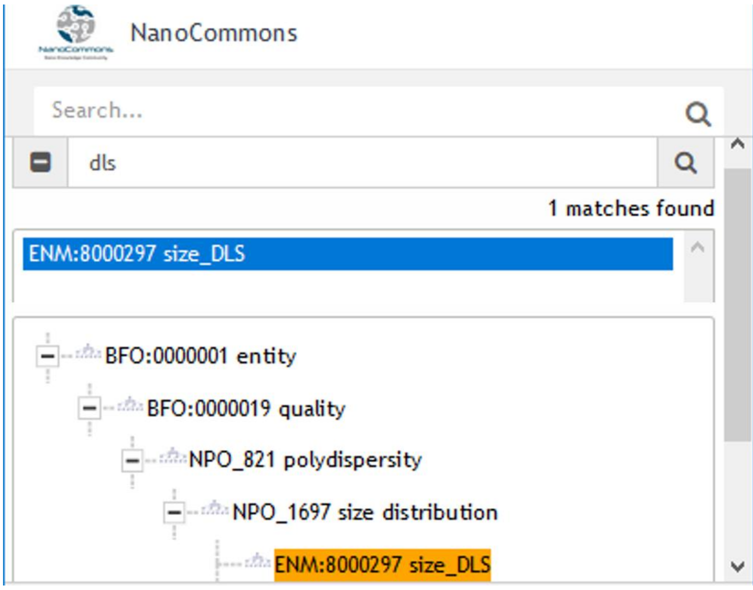

Figure 6. Keyword search in the ontology browser here for term "dls" returns matches in any of the >20 ontologies integrated into the NanoCommons portal.

A suite of tools is also being developed to perform semi-automatic annotation and concept recognition in free text sources. The method uses standard Natural Language Programming (NLP) tools to extract mentions of concepts, then employs algorithms which improve upon those described in the text mining literature, to determine the context of the concept, and its relationship with other surrounding concepts. The toolset also includes a web-based validation tool, which allows an expert to check the results of the extraction process. The results can be downloaded for further analysis, and feedback integrated into the extraction system to improve performance. The software also supports plugins, and such a plugin could upload validated and corrected data to a database at the end of the validation process.

These tools will be employed both for the purposes of extracting background knowledge on physiochemical characterisation and toxicity of NMs from academic papers, and for annotating information from free-text components of omics analyses following molecule exposure to NMs. Part of these datasets have already been manually annotated by experts, this forming a source for automated validation of the extraction.

Dissemination Activities

Ontology meetings

1st NanoCommons Hackathon on "Ontological Annotation of Datasets"

This event[2], organised jointly with OpenRiskNet, took place on 9 October 2018 in Athens (Greece), in conjunction with the NanoCommons Consortium Meeting and the OpenTox Euro Conference, provided participants with an introduction to using ontologies. See Appendix 3 for the full agenda and Deliverable D2.1: 1st Annual conference and nano-exploitation day, stakeholder workshop and User call for a more analytical description of the workshop.

During the event, presentations on ontologies were given by Anastasios Papadiamantis (UoB, title: "What is an Ontology") and Luke Slater (UoB, title: "How eNM ontology works"), and the Biomax ontology browser and KB was introduced by Dieter Maier (Biomax, title: "NanoCommons KnowledgeBase intro"). The presentations were followed by a hands-on hackathon, during which the participants searched through established ontologies (e.g. eNanoMapper Ontology) and annotated a model dataset provided by the NanoCommons project that originated from data produced and curated within the FP7 NanoMILE project. The participants also learned how to prepare electronic files (e.g. tab-delimited, Excel, XML) containing the raw data and the ontological metadata to support data upload into the database. The event was attended remotely by members of the Center for Sustainable Nanotechnology (CSN, USA; https://susnano.wisc.edu/) who are also adopting the NanoCommons approach for the management of the large amounts of data being generated in their multi-institute multi-year centre.

OpenRiskNet/NanoCommons ontology meeting

This event was organised jointly with the OpenRiskNet e-infrastructure project on 13-14 December 2018, in Brussels (Belgium)[3].

The goal of this meeting was to get a picture of the ongoing ontology activities in the area of toxicology, to harmonize these efforts and the developed ontologies therein, and to extend the existing toxicology ontology to support NanoCommons and OpenRiskNet tasks. One main focus was on the ontological annotation of Application Programming Interfaces (APIs) as already used on the OpenRiskNet reference infrastructure (https://home.prod.openrisknet.org/) and currently adopted by NanoCommons data, modelling and risk assessment services offered to Users via the Transnational Access programme. Other goals included the organization of identification of missing terms and required ontology extensions, as well as to write up guidance documents to create more specific ontology terms and clear definitions. These recommendations already guided the ACEnano ontology work described above. Figure 7 shows the highlights of the ontology workshop agenda.

[2] https://www.nanocommons.eu/1st-nanocommons-hackathon-ontological-annotations-of-datasets/
[3] https://openrisknet.org/events/45/

Topics:

1. What ontologies are out there and can we combine them to a toxicology application ontology.

2. Data and software schema: How much ontology do we need to annotate complex services.

3. Ontology Hacking.

Figure 7. Summary agenda for the OpenRiskNet/NanoCommons ontology workshop.

Tutorials

Various tutorials have been developed to support dissemination of the ontology among the other NanoSafety Cluster projects. The source code for these tutorials is available from GitHub, mostly as Markdown files (16):

- New: *Adding ontology terms*
  - Source: https://github.com/enanomapper/tutorials/tree/feature/descriptorTerms/Added%20ontology%20terms
- New: *Adding ontology terms for Nanomaterial Descriptors*
  - Source: https://github.com/enanomapper/tutorials/tree/feature/descriptorTerms/Descriptor%20Terms
- Updated: *Browsing the eNM ontology with BioPortal, AberOWL and Protégé*
  - Source: https://github.com/enanomapper/tutorials/tree/feature/descriptorTerms/BrowseOntology
- New: *Adding nanomaterial data*
  - Source: https://github.com/NanoCommons/tutorials/blob/master/enteringData/index.md

Furthermore, several of these tutorials have been semantically annotated with BioSchemas (https://bioschemas.org) annotation , in close collaboration with the ELIXIR Toxicology Community (https://github.com/egonw/ELIXIR-Tox). This annotation allows the ELIXIR TeSS system to automatically pick up updated versions of these tutorials (17). Furthermore, the TeSS system makes the tutorials findable with its European-wide search engine. Tutorials are grouped under the following content providers:

- https://tess.elixir-europe.org/content_providers/enanomapper
- https://tess.elixir-europe.org/content_providers/nanocommons

Transnational Access (TA) Projects

In the first round of applications for TA, two applications have been submitted to visit the Maastricht University partner to work on using the eNanoMapper ontology for their use cases. Following their positive evaluation and selection for TA funds, these projects will take place in autumn 2019. The aim of the submitted applications were:

1. To get relevant training and acquire knowledge on the annotation of publicly available ENM characterisation and nanosafety data, identifying the correct terms for annotation, add missing terms into the eNanoMapper ontology and improve/add existing/missing definitions. The outcome from this TA project will be a set of additional (minimum 50) new ontological terms added to the NanoCommons ontology.
2. Use of ontological annotation to improve data FAIRness, via the improvement of the Resource Description Framework (RDF) output of eNanoMapper datasets with annotated entries, query semantic databases using ontology hierarchies and learn how to configure files for eNanoMapper database import that is completely aligned to the NanoCommons knowledgebase allowing direct interoperability. The output from this TA project will be a minimum of 3 datasets on different aspects of NMs safety demonstrated as being fully interoperable across eNanoMapper database and the NanoCommons KnowledgeBase.
3. To develop ontologies and template formats for presenting and storage of nanosafety relevant data obtained by molecular modelling methods, such as molecular dynamics or quantum-chemical computations, in accordance with the requirements of the European Commission, and fully aligned with and extending the templates and ontologies developed by the EMMC.

Plans for 2019-2020

Slimmer and ROBOT

The current Slimmer tool used for the development of the ontology (1) is a custom tool based on the OWLAPI library (8). While the OWLAPI library is very powerful, it has not always been easy to use. Particularly, extracting predicates for use in the eNanoMapper ontology turned out to be a difficult issue. In the following months the eNanoMapper Slimmer tool will be rewritten to use the ROBOT library (18). This will ensure that the build server is more flexible and will benefit from developments from other related consortia, e.g. the OBO Foundry community, managing ontologies like the Gene Ontology.

Updated and improved term description handling

The current ontology still lacks descriptions for many terms. This can be partly explained by descriptions being stored in the third-party ontologies with a variety of predicates and not all descriptions are copied into the eNanoMapper ontology correctly. A second problem is that the upstream, third-party ontologies do not have term descriptions. We plan to work with the upstream ontology community to add missing descriptions.

Report extensions to upstream, third-party ontologies

The eNanoMapper ontology has extensions for various other ontologies, particularly the BAO (19) and the NanoParticle Ontology (NPO) (20). There is communication with these upstream, third-party ontologies, but not all content has been applied upstream yet. This will be picked up again.

Roadmap towards a community approach to the NanoSafety ontology

There is a clear need to develop a roadmap to support the transition of the eNanoMapper ontology into a NanoSafety community ontology approach similar to that adopted by the Gene Ontology (GO) (21). Building on lessons learned from the GO on how the collaborative community-driven ontology evolution is implemented in the real-life practical setting in terms of successes and challenges for the approach, a roadmap will be developed together with the modelling and governance cluster of projects to support the establishment of a community driven ontology development for NanoSafety.

Conclusions

The NanoCommons project has taken over the release management and continued development of the eNanoMapper ontology, albeit with significantly less resources than were available for the initial development and implementation. NanoCommons has made two major releases of the ontology in a period of 18 months, made a number of important initial updates to the development platform that are important steps towards facilitating a community and consensus driven ontology building, and outlined a work plan for the next period. The two major releases increased the coverage of the ontology, based on the needs identified from other NanoSafety Cluster projects and efforts, like Nanoreg2, Gracious, ACENano, the U.S.A. NIKC project, and the Malta Initiative. Collectively, these releases have added 1805 new terms to the ontology.

Additionally, many interactions with other projects working on nano-related or nano-specific ontologies or ontology extensions have been initiated and strengthened by the outreach and disseminations activities. This will be continued and even more intensified by developing and executing a roadmap towards a community approach towards a general NanoSafety ontology integrating all projects of the NanoSafety Cluster with ontology tasks as well as international initiatives.

Acknowledgements

We thank the nanosafety community who contributed to this effort by requesting terms and giving feedback. This includes Dr. Nina Jeliazkova (Nanoreg2, Gracious), Dr. Geert Cornelis (ACEnano), Prof. Susana Loureiro and her group at the University of Aveiro, Prof. Richard Handy and the members of the NanoFASE and NanoFARM consortia.

Abbreviations

AOP	Adverse Outcome Pathway
API	Application Programming Interface
BAO	BioAssay Ontology
BFO	Basic Formal Ontology
CHEMINF	Chemical Information Ontology
EU	European Union
FABIO	FRBR-aligned Bibliographic Ontology
FP7	Framework Programme 7
H2020	Horizon 2020 Programme
NIKC	NanoInformatics Knowledge Commons
NLP	Natural Language Programming
NPO	NanoParticle Ontology
OECD	Organisation for Economic Co-operation and Development
OWL	Web Ontology Language
OWLAPI	Library that provides an API to OWL
ROBOT	A command-line tool for working with ontologies
SIO	Semanticscience Integrated Ontology
TA	Transnational Access

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Appendix 1: Details from BioPortal

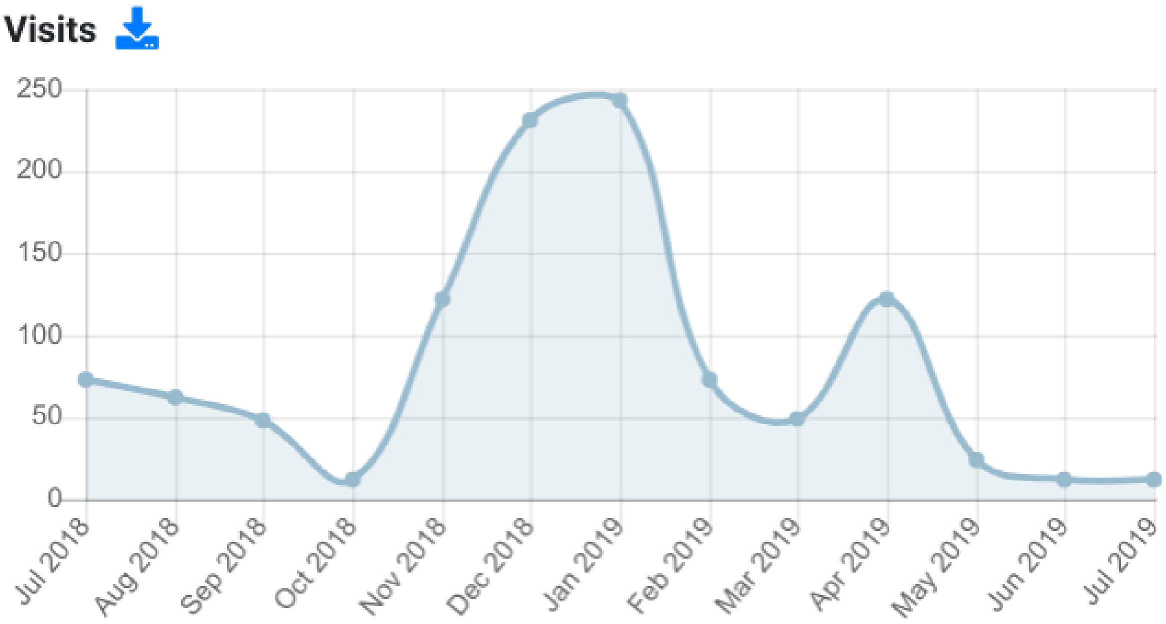
Release overview

Submissions

Version	Released	Uploaded	Downloads
5.0.2 (Parsed, Indexed, Metrics, Annotator)	09/27/2018	07/27/2019	OWL | CSV | RDF/XML | Diff
5.0.1 (Archived)	09/27/2018	09/27/2018	OWL | Diff
5.0 (Archived)	09/14/2018	09/14/2018	OWL | Diff
5.0 (Archived)	09/13/2018	09/13/2018	OWL | Diff
4.1 (Archived)	10/11/2017	10/11/2017	OWL | Diff

more...

Download Statistics



Appendix 2: Required new ontology terms prepared for integration into eNanoMapper ontology

No	ACEnano Term Needed In ENM Ontology	Ontology In Which Term Is Found	Ontology URL Of Term	Ontology Description of Term	NanoCommons Specialists Description
1	Addition of chemicals	NA	NA	NA	1.NA, 2. We use 'spiking' instead of addition
2	Amplitude	National Cancer Institute Thesaurus (NCIT)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C70831	The magnitude of an oscillation.	This is context dependant as there are several different "types" of amplitude
3	Aqueous liquid	NA	NA	NA	A solution in water (ammonium barcarbonate made up in water, as opposed to methanol)
4	Assay-on-a-chip	NA	NA	NA	NA
5	Asymmetrical field flow fractionation	NA	NA	NA	NA
6	Average size dimension	NA	NA	NA	NA
7	Biological tissues	NA	NA	NA	1.A collections of cells and extracellular matrix from the same origin/organ that carry out a specific function; 2.Tissue sample from any living being - always useful to state from which organism and organ
8	Brunauer–Emmett–Teller analysis	NA	NA	NA	Technique used to determine the surface area of solid particles
9	Calibrated Volume Pipettor- perhaps erase it from KI	NA	NA	NA	1.Synonym of pipette; 2.We do not use anything else than non calibrated pipettes (and we don't use the term pipettor)
10	Cells	Medical Subject Headings (MESH)	http://purl.bioontology.org/ontology/MESH/D002477	The smallest units of living structure capable of independent existence, composed of a membrane-enclosed mass of protoplasm and containing a nucleus or nucleoid.	The most basic biological unit of a living organism
11	Centrifugal field flow fractionation	NA	NA	NA	NA
12	Centrifugal Field-Flow Fractionation-MALS	NA	NA	NA	NA
13	Chloride concentration	NA	NA	NA	NA
14	CO2 concentration	NA	NA	NA	NA
15	Column test	NA	NA	NA	NA
16	Compound	National Cancer Institute Thesaurus (NCIT)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C43366	A substance formed by chemical union of two or more elements or ingredients in definite proportion by weight.	A chemical substance composed of two or more elements
17	Conductivity	National Cancer Institute Thesaurus (NCIT)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C134263	A measure of the ion-facilitated electron current through a material.	NA
18	Cuvettes	FAST (Faceted Application of Subject Terminology) Topical Facet (FAST-TOPICAL)	http://id.loc.gov/authorities/subjects/sh85035015	NA	1.Receptical for liquids for spectrophometric analsysis; 2.Cuvettes is again a very divers term - describing them for different kind of applications (photometric, chemistry etc.) as well as being from very different materials (e.g. plastic, glass)
19	Density matching of fluid	NA	NA	NA	NA
20	Deposition rate	NA	NA	NA	NA
21	Dialysis + ICP-MS	NA	NA	NA	NA
22	Dilution	NA	NA	NA	Reduction in concentration of an analyte

23	Dilution scale factor	NA	NA	NA	1.The degree to which the concentration of a analyte has been reduced, 2.We only use dilution factor
24	Disc centrifuge	NA	NA	NA	NA
25	Disposable cuvettes	NA	NA	NA	1.Non reusable cuvettes (Typically plastic rather than Quartz); 2.Usually used for photometry (e.g. optical density reading) and consist of plastic
26	Dissolved organic carbon/surfactants	NA	NA	Na	NA
27	DLS intrument	NanoParticle Ontology (NPO)	http://purl.bioontology.org/ontology/npo#NPO_1766	An instrument which is used to perform dynamic light scattering technique.	Particle sizing technique based on Brownian motion and scattered light
28	Dye loaded field flow fractionation	NA	NA	NA	NA
29	Electrophoretic mobility	NanoParticle Ontology (NPO)	http://purl.bioontology.org/ontology/npo#NPO_1315	Mobility of a charged particle in electrophoresis, measured as the rate of migration (usually in cm/s) per unit electric field strength (usually V/cm) of the charged particle.	Migration of analytes under an electric field through a conductive liquid
30	Elemental composition and chemical purity	NA	NA	NA	1.NA, 2.Agree, and we give details of either the purity (e.g. 99 %) and/or what the impurities are (composition as well as percentage)
31	Energy Dispersive X-ray Spectroscopy in the SEM and TEM	NA	NA	NA	Chemical analysis method that relies on X-ray excitation of the sample
32	Extractant	NA	NA	NA	NA
33	Extraction	Chemical Methods Ontology (CHMO)	http://purl.obolibrary.org/obo/CHMO_0001577	The transfer of a solute from a liquid phase to another immiscible or partially-miscible liquid phase in contact with it.	The isolation of analytes from an undesiered matrix
34	Filtration	National Cancer Institute Thesaurus (NCIT)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C16583	The process of passing a liquid or gas through a filter.	A mechanistic, biological or physical process by which solids are separated from liquids (or gases) by adding a barrier that only the fluid can pass through/that the solids of a defined size or property cannot
35	Force tensiometry	NA	NA	NA	NA
36	Freeze-drying	National Cancer Institute Thesaurus (NCIT)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C28150	A dehydration process typically used to preserve a perishable material. The specimen is frozen and then dehydrated at low temperature in a high vacuum.	A low temperature, low pressure dehydraition technique
37	Freezing	National Cancer Institute Thesaurus (NCIT)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C48160	The act or event which causes the transition from a liquid to solid matter phase.	Reducing the temperature of a liquid to the temperature at which its phase transforms from liquid to solid
38	Full field transmission X-ray microscopy	NA	NA	NA	NA
39	Homoaggregation rate	NA	NA	NA	The rate of the transfer of aggregates from the bin (size interval) of smaller particle size to the bin of larger particle size.
40	Hydrophobic interaction chromatography	NA	http://localhost/plosthes.2017-1#1177	NA	NA
41	Hydrophobicity	National Cancer Institute Thesaurus (NCIT)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C63813	The inherent characteristic of a molecule or substance to be immiscible in water. The property means that the moiety of interest does not dissolve in, absorb, or mix easily with water.	A property of a molecule describing its propensity to associate with neutral or non-polar solvents or molecules as opposed to polar ones
42	Interfering components or isotope	NA	NA	NA	NA
43	Ion-selective electrode	Chemical Methods Ontology (CHMO)	http://purl.obolibrary.org/obo/CHMO_0002393	An electrode which responds to the activity of a primary ion in presence of various other (interfering) ions in the sample solution. Ion-selective electrodes contain a selective membrane which contains fixed or mobile sites that interact with ions in solution.	NA
44	Ionic strength	National Cancer Institute Thesaurus (NCIT)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C52478	The weighted concentration of ions in solutions.	NA
45	Laser induced breakdown	Chemical Methods Ontology (CHMO)	http://purl.obolibrary.org/obo/CHMO_0000258	A type of atomic emission spectrometry where a high energy laser pulse is used	NA

	detection			to generate a plasma which acts as the excitation source.	
46	Limit of Quantification- must be added in KI! Or add "Lower limit of detection" to eNM?	Chemical Methods Ontology (CHMO)	http://purl.obolibrary.org/obo/CHMO_0002802	The smallest measure that can be quantified with reasonable certainty for a given analytical procedure.	Limit of quantification is the value which gives you the lowest, reliable quantifiable amount of a compound
47	Lowest limit of detection	National Cancer Institute Thesaurus (NCIT)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C105701	The smallest concentration of an analyte that can be determined with a stated precision or confidence.	1.The smallest value measurable using a defined method; 2.Limit of quantification should be added, limit of detection is not quantitative but qualitative
48	MALS/SLS	NA	NA	NA	NA
49	Malvern Zetasizer	NA	NA	NA	Equipment to perform DLS and zeta potential analyses
50	Mastersizer	NA	NA	NA	NA
51	Matrix-Assisted Laser Desorption/Ionization	National Cancer Institute Thesaurus (NCIT)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C48040	soft ionization technique which produces quasimolecular ions of large organic molecules up to several 100 kDa molecular mass.	NA
52	Medium	NanoParticle Ontology (NPO)	http://purl.bioontology.org/ontology/npo#NPO_1853	A fluid which can hold other substances in solution or in suspension.	The solute in which a sample is dilution or exposed to
53	Milling	NA	NA	NA	The use of rotational cutting or grinding to reduce the size of a bulk material
54	Nanoparticle Tracking Analysis	NA	NA	NA	Particle sizing technique based on Brownian motion and scattered light
55	NP-cell interaction	NA	NA	NA	NA
56	Nuclear magnetic resonance spectroscopy relaxation	NA	NA	NA	NA
57	O2 concentration	NA	NA	NA	NA
58	Osmotic concentration	NA	NA	NA	NA
59	Other particles	NA	NA	NA	NA
60	Parameters	National Cancer Institute Thesaurus (NCIT)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C80474	Technical specifications about a device that are issued by the manufacturer.	Characteristic defining or classifying factor for a particular system
61	Particle shape	NA	NA	NA	The geometric profile of a nanoparticle
62	pH	NanoParticle Ontology (NPO)	http://purl.bioontology.org/ontology/npo#NPO_1814	A dimensionless concentration notation which denotes the acidity of a solution in terms of activity of hydrogen ions (H+).	An expression of acidity or basicity of a solution, defined as the concentration of hydrogen ions per litre
63	Phase	NanoParticle Ontology (NPO)	http://purl.bioontology.org/ontology/npo#NPO_1610	A substance or a portion of a substance, which has uniform physical and chemical properties.	Distinctive state of a material such as solid, liquid, gas or plasma
64	Phosphate concentration	NA	NA	NA	NA
65	Pipettes	PLOS Thesaurus (PLOSTHES)	http://localhost/plosthes.2017-1#7339	NA	1.Handheld equipment to precisly aliquot liquids; 2.They come in very different shapes with different levels of accuracy from single glass pipettes, to adjustable or even electronic and multichannel pipettes - it might be useful to always state the name and scale and level of accuracy together with the term pipette
66	Pipettors- perhaps erase it from KI	NA	NA	NA	1.Synonym of pipette; 2.I had to look up the difference between pipette and pipettor (we don't use the latter)
67	Pore size	National Cancer Institute Thesaurus (NCIT)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C112332	A quantitative or qualitative measurement of the physical dimensions of the pores in a material.	Diameter of pore
68	Powder	National Cancer Institute Thesaurus (NCIT)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C45302	A solid substance in the form of tiny loose particles; a solid that has been pulverized.	A dry bulf solid composed of fine particles
69	Preferential orientation	NA	NA	NA	NA

70	Purity (resistivity)	National Cancer Institute Thesaurus (NCIT)	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.	NA
71	Quartz crystal microbalance with dissipation monitoring	NA	NA	NA	NA
72	Raw data	National Cancer Institute Thesaurus (NCIT)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C142663	The original information, collected from the primary source.	Unprocessed data (i.e. unnormalised, prior to fourier transformation)
73	Redox speciation	NA	NA	NA	NA
74	Scanning Transmission Electron Microscope-Energy-dispersive X-ray spectroscopy	NA	NA	NA	Technique to provide elemental composition. A focused beam of electrons is formed that is scanned over the sample from the upper-left to lower-right pixels of a specimen while some desired signal is collected to form an image. STEM-EDX is STEM coupled with an EDX detector.
75	Scanning transmission X-ray microscopy	NA	NA	NA	NA
76	SEC/HDC/HIC	NA	NA	NA	NA
77	Single Particle Inductively Coupled Plasma Mass Spectrometry	NA	NA	NA	NA
78	Single Particle Time of flight Inductively Coupled Plasma Mass Spectrometry	NA	NA	NA	NA
79	Single-cell Single Particle Inductively Coupled Plasma Mass Spectrometry	NA	NA	NA	NA
80	Small-Angle X-ray Scattering	Chemical Methods Ontology (CHMO)	http://purl.obolibrary.org/obo/CHMO_0000204	A method for determining structure by measuring the change in direction or energy of X-rays scattered by a sample at low angles (0--10 deg.).	NA
81	Solid matrix	NA	NA	NA	NA
82	Speed	National Cancer Institute Thesaurus (NCIT)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C41146	A scalar measure of the rate of movement of the object expressed either as the distance travelled divided by the time taken (average speed) or the rate of change of position with respect to time at a particular point (instantaneous speed).	Magnitude of velocity
83	Storage temperature	National Cancer Institute Thesaurus (NCIT)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C101707	The recommended storage temperature for a device.	1.The optimal temperature at which samples should be stored (usually with the caveat of maximum time the sample is stable at given temperature); 2.Temperature an entity is stored at, mostly goes together with the storage conditions (e.g. stored dark at 4 degree C in a fridge)
84	Suspension	NanoParticle Ontology (NPO)	http://purl.bioontology.org/ontology/npo#NPO_532	A mixture in which fine particles are suspended in a fluid where they are supported by buoyancy.	Heterogenous mixture of solids in solution with sufficient size to sediment but not dissolve in the solute
85	Thermogravimetric analysis coupled with IR-GC or MS	NA	NA	NA	Samples can be heated under inert gas (N2) or pyrolysed (air) at selected temperatures to monitor the gases evolved. The infrared spectrometer is ideal for identifying CO2, while the GCMS is well suited to identify volatile organic compounds (VOCs)
86	Time of flight secondary ion mass spectrometry	Chemical Methods Ontology (CHMO)	http://purl.obolibrary.org/obo/CHMO_0000565	Mass spectrometry where the sample is bombarded with a stream of primary mass-selected particles and the secondary ions ejected from the sample are detected by accelerating them to the same (known) kinetic energy and measuring the time taken for each ion to reach a detector at a known distance. This time is dependent on the mass-to-charge ratio of the ion.	NA

87	Time resolved Dynamic Light Scattering	NA	NA	NA	NA
88	Time resolved nanoparticle tracking analysis	NA	NA	NA	NA
89	Time resolved Single Particle Inductively Coupled Plasma Mass Spectrometry	NA	NA	NA	NA
90	Tip Enhanced Raman Scattering (nano-Raman)	Chemical Methods Ontology (CHMO)	http://purl.obolibrary.org/obo/CHMO_0000678	Spectroscopy where the Raman scattering of monochromatic light, from a visible laser (500--650 nm), by metal surfaces, where scattering is enhanced by the optical near-field of a metal-coated scanning probe microscopy tip, is detected.	NA
91	Transmission electron microscopy with electron energy loss spectroscopy	Chemical Methods Ontology (CHMO)	http://purl.obolibrary.org/obo/CHMO_0000373	Spectroscopy where a beam of electrons with a known, narrow range of kinetic energies is transmitted through a sample and the energy distribution of the transmitted electrons is measured.	TEM coupled with an EELS detector. Electron energy loss spectroscopy (EELS) involves measuring energy loss dispersion of inelastically scattered high-energy electrons transmitted through a thin sample.
92	Ultracentrifugation + ICP-MS	NA	NA	NA	NA
93	Ultrafiltration + ICP-MS	NA	NA	NA	NA
94	Upper limit of detection	NA	NA	NA	The largest value measurable using a defined method
95	UV-Vis Spectrophotometer	Eagle-I Research Resource Ontology (ERO)	http://purl.obolibrary.org/obo/ERO_0000895	A spectrophotometer which measures emissions in the ultraviolet-visible spectral region.	Instrument to determine UV-Vis
96	Viscosity	National Cancer Institute Thesaurus (NCIT)	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C75912	The resistance of a liquid to sheer forces and flow.	NA
97	Water concentration	NA	NA	NA	NA
98	Wide-Angle X-ray Scattering	Chemical Methods Ontology (CHMO)	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.	NA
99	X-ray absorption near edge spectroscopy	NA	NA	NA	NA
101	X-Ray Diffraction - crystalline phase	NA	NA	NA	NA
101	X-Ray Diffraction - crystallite size	NA	NA	NA	NA
102	X-Ray photon spectroscopy	Chemical Methods Ontology (CHMO)	http://purl.obolibrary.org/obo/CHMO_0000404	Spectroscopy where the sample is illuminated with X-rays causing ionisation and the emission of photoelectrons, the energies of which are measured.	Elemental and chemical state information about the surface of solid material sample. The incident x-rays cause photoelectrons to be emitted from the surface and the kinetic energy of these emitted electrons is characteristic of the element from which the photoelectron originated.

Appendix 3: Ontological hackathon agenda

Agenda

Time	Title	Presenter(s)
15.30-15.45	What is an Ontology?	Iseult Lynch, Anastasios Papadiamantis (UoB)
15.45-15.55	How eNM ontology works	Luke Slater (UoB)
15.55-16.15	Annotation Procedure	All
16.15-16.25	NanoCommons KnowledgeBase intro	Dieter Meier (BIOMAX)
16.25-17.25	Groups work on subset of dataset	All
17.25-17.45	Groups present to each other their work while DB team uploads the results to NanoCommons KnowledgeBase	All
17.45-18.00	Discussion and final comments	All