DELIVERABLE REPORT D2.4

Ontology final release

GRANT AGREEMENT:	604134
ACRONYM:	eNanoMapper
NAME:	eNanoMapper - A Database and Ontology Framework for Nanomaterials Design and Safety Assessment
PROJECT COORDINATOR:	Douglas Connect GmbH
START DATE OF PROJECT; DURATION:	1 February 2014; 36 months
PARTNER(s) RESPONSIBLE FOR THIS DELIVERABLE:	DC

DATE:	31 January 2017
VERSION:	V.1.0

Call identifier	FP7-NMP-2013-SMALL-7
Document Type	Deliverable Report
WP/Task	WP2 / Tasks 2.5, 2.6 and 2.7
Document ID	D2.4 Ontology final release
Status	Draft

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Purpose of the Document	T2.5 T2.6 and T2.7
Document History	First draft, 24/01/2017

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GLOSSARY

Abbreviation / acronym	Description
ECHA	European Chemical Agency
eNM	eNanoMapper
ISO	Internaltional Organization for Standadization
JRC	Joint Research Centre
NECID	Nano Exposure & Contextual Information Database
NPO	NanoParticle Ontology
OECD	The mission of the Organisation for Economic Co-operation and Development
OWL	Web Ontology Language
RDF	Resource Description Framework
SPARQL	Simple Protocol and RDF Query Language
WG	Working Group
WP	Work Package

1. EXECUTIVE SUMMARY

The eNanoMapper project aims to build an ontology and database to collate and describe data relevant for “safety by design” engineered nanomaterial development. Work Package 2 of this effort is developing and disseminating a comprehensive ontology for the nanosafety domain, encompassing nanomaterials and all information relating to their characterization, as well as relevant experimental paradigms, biological interactions and safety information. This deliverable report describes the work undertaken for the final release of the ontology (Task 2.7), including the internal (Task 2.5) and external review (Task 2.6), and the technical and curatorial processes that have been followed to create it.

2. INTRODUCTION

Following the first release the eNanoMapper ontology (reported in Deliverable Report D2.3), internal and external review processes led to feedback from eNM partners and from members of other European nanosafety projects (e.g. NANoREG, NECID, and NANOMILE). This directed our subsequent work to both enlarge the ontology and to improve its framework. Just as for the initial release of the ontology, the majority of the new terms added to the ontology for the enhancement work were reused from existing ontologies using the automated scripting process described previously, while some terms needed to be manually curated by the eNanoMapper team. This review-feedback-enhancement process was used for the development of two further intermediate releases of the ontology (September 2015 and March 2016) and for the final release in January 2017.

3. FINAL ENM ONTOLOGY RELEASE

3.1 User metrics of the eNM Ontology

eNM ontology version	Release Date	Number of Terms	External ontologies reused
1.0	11/03/2015	7260	11
2.0	14/09/2015	6811	15
3.0	01/03/2016	8407	19
4.0 (Final)	26/01/2017	10881	22

Table 1: Metrics of the eNM Ontology as calculated by BioPortal

Of the 10,881 terms in the final release (v4.0), 10,295 were reused from 22 other ontologies in the biomedical domain. The remaining 586 terms were not present in existing ontologies and so were created manually; the majority of these (321) were created after release 3.0.

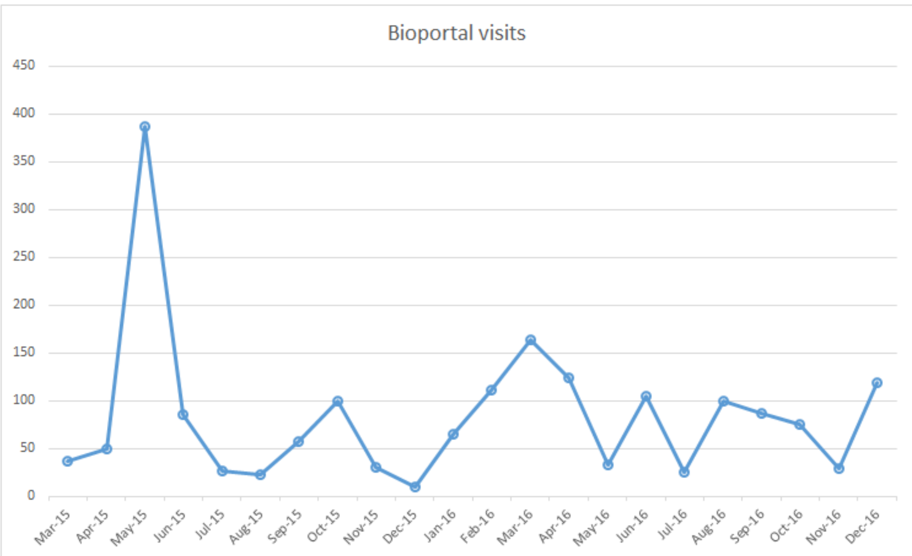


Figure 1: Number of visits to the eNM Ontology on BioPortal

3.2 Internal and external reviewing of the eNM Ontology

3.2.1 Ontology internal review process

3.2.1.1 Issue Tracker within GitHub for internal review

An "ontologies" repository was created within the "enanomapper" project page within GitHub. Within this specific repository an Issue Tracker was created in order to track modification requests applicable to the eNanoMapper ontology. As can be seen in Figure 1 until now, 99 issues were filed of which 76 have been closed. The majority of these requests have been made by eNM project partners. The requested modification involved changing the overall structure and organisation of the ontology, adding additional terms in order to increase the coverage for the respective domain, addition extra descriptive information or axioms to terms etc.

All of these requests were handled with care by the ontology curation team which has led to improved releases of the eNM ontology.

3.2.1.2 Feedback from hackathons

During several hackathons between the eNM partners numerous issues were discussed considering the content and structure of the ontology. Substantial numbers of ontological terms were manually added following these sessions. In addition several requests were made by the database team in order to facilitate the data uploading process with ontology-tagged template files. An example is the extensive set of templates of the NANoREG project.

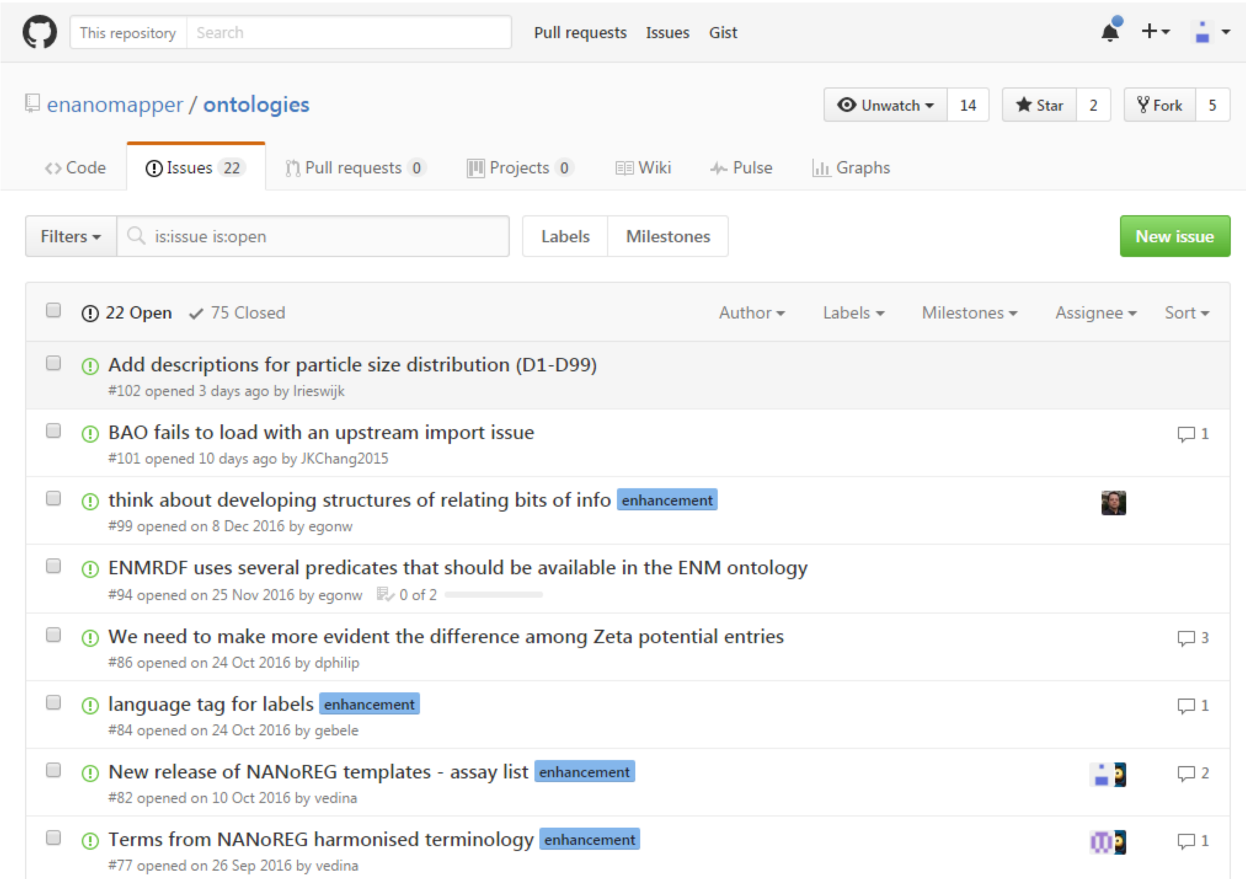


Figure 2: The open source online "ontologies" Issue Tracker on GitHub

3.2.2 Ontology external review process

3.2.2.1 Issue Tracker within GitHub for external review

Modification requests from collaborators outside the project were also made via the Issue Tracker of GitHub (see Figure 2). Over the period of the project 97 issues have been opened of which 75 have been addressed and 22 issues are still unresolved. All issues are annotated with tags indicated the issue is a feature request ("enhancement") or problem ("bug"). Comments can be added to provide further information or ask question, as is used in the issues shown in FIg. 2 as visible by the text balloons on the right side. Issues can be assigned to people to indicate who the next person is to take action.

3.2.2.2 Input from members of the nanosafety community

On the 8th of December 2016 the eNM Ontology was presented during a webinar to the US-based Nanotechnology Working Group (Nano WG). Afterwards the ontology curation team received feedback from members of the nanosafety community regarding the composition of the ontology. The comments received focussed mainly on the complexity and the use of the ontology by different end-users. An example was given for zeta potential, which was followed up using the Issue Tracker on GitHub.

3.2.2.3 Feedback by other closely related nanosafety projects

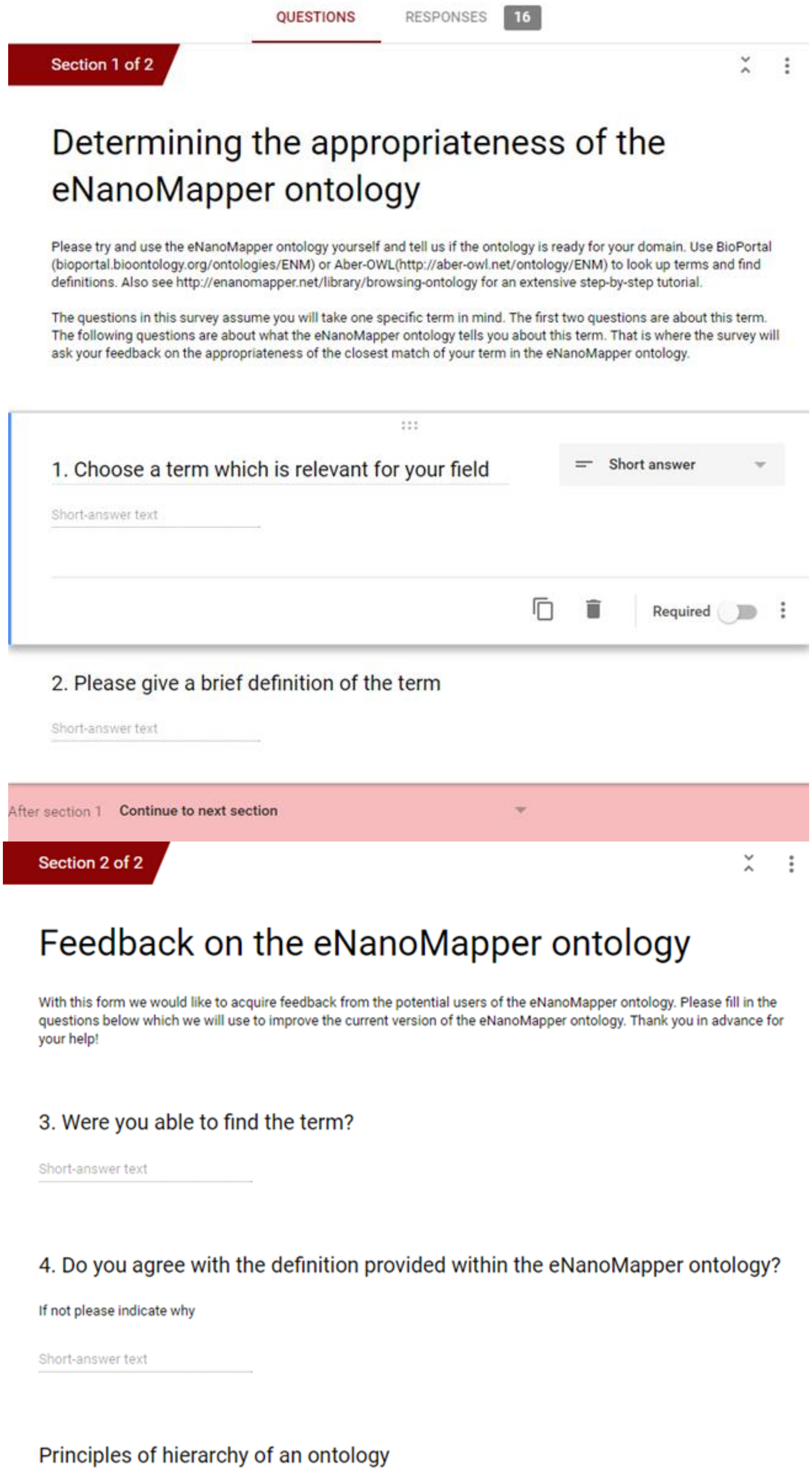
During the course of the project the ontology curation team has had several meetings with members of other European nanosafety projects such as NANoREG, NECID and NANOMILE. During these sessions an introduction was given to the project in general and more specifically on the database and the ontology. In parallel a tutorial was provided in which the use and accessibility of the ontology via online repositories (e.g. BioPortal, Aber-OWL or Ontology Lookup Service) or locally (using Protégé) was shown. The purpose of these sessions was to stress the importance of an harmonizing ontology within the nanosafety domain but also to encourage database owners and developers to use the ontology within their own database. Following existing templates and database schemas from these respective projects new terms were added to the eNM Ontology either through re-using existing ontological terms or creating new ones.

3.2.2.4 Survey on the appropriateness of the eNM ontology

In order to evaluate whether users were in agreement with the composition, structure and appropriateness of the eNM Ontology, a survey was created using Google Forms (see Figure 2). Within the survey the following questions were asked:

1. Choose a term which is relevant for your field
2. Please give a brief definition of the term
3. Were you able to find the term?
4. Do you agree with the definition provided within the eNanoMapper ontology?
5. Do the super classes make sense to your field (if applicable)?
6. Do the sub classes make sense to your field (if applicable)?
7. Do you agree with the logical structure leading towards the term of interest?
8. Additional comments

The survey was used during the meeting with NECID on the 3rd of March 2016 in Leiden (The Netherlands), the hackathon on Ontology for Modelling & Nano-Descriptors on the 11th of April 2016 and also during the interactive session on Nano Ontologies which was part of the “Enabling a sustainable harmonised knowledge infrastructure supporting nano environmental and health safety assessment” workshop on the 24th of October 2016 in Rheinfelden (Germany). In total 16 participants of either of these sessions filled in the survey as can be seen in Annex 6.1. From this questionnaire we could conclude that people were in general able to find specific terms of interest but often these were lacking an appropriate description or definition. In addition some people indicated that some of the super and subclasses were not in the correct place and should therefore be changed. A lot of these comments also ended up within the Issue Tracker of the ontologies repository on GitHub.



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Section 1 of 2

Determining the appropriateness of the eNanoMapper ontology

Please try and use the eNanoMapper ontology yourself and tell us if the ontology is ready for your domain. Use BioPortal (bioportal.bioontology.org/ontologies/ENM) or Aber-OWL(http://aber-owl.net/ontology/ENM) to look up terms and find definitions. Also see http://enanomapper.net/library/browsing-ontology for an extensive step-by-step tutorial.

The questions in this survey assume you will take one specific term in mind. The first two questions are about this term. The following questions are about what the eNanoMapper ontology tells you about this term. That is where the survey will ask your feedback on the appropriateness of the closest match of your term in the eNanoMapper ontology.

1. Choose a term which is relevant for your field

Short answer

Short-answer text

Required

2. Please give a brief definition of the term

Short-answer text

After section 1 Continue to next section

Section 2 of 2

Feedback on the eNanoMapper ontology

With this form we would like to acquire feedback from the potential users of the eNanoMapper ontology. Please fill in the questions below which we will use to improve the current version of the eNanoMapper ontology. Thank you in advance for your help!

3. Were you able to find the term?

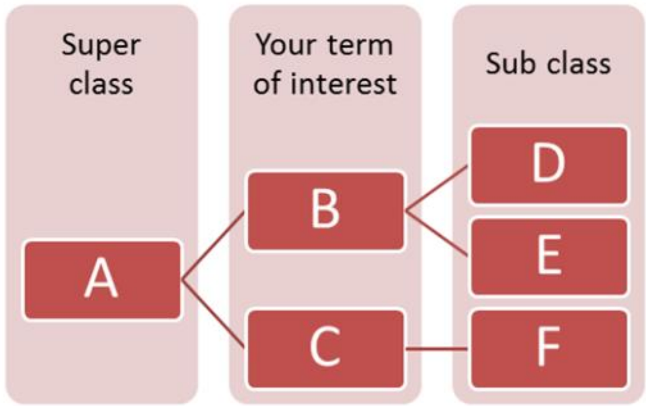
Short-answer text

4. Do you agree with the definition provided within the eNanoMapper ontology?

If not please indicate why

Short-answer text

Principles of hierarchy of an ontology



5. Do the super classes make sense to your field (if applicable)?

A super class is a class from which your term of interest is derived

Short-answer text

6. Do the sub classes make sense to your field (if applicable)?

A sub class is a class which is derived from your term of interest

Short-answer text

7. Do you agree with the logical structure leading towards the term of interest?

Short-answer text

8. Additional comments

Long-answer text

Figure 3: Survey on the evaluation of the appropriateness of the eNM Ontology (created within Google Forms)

3.3 Use of the eNM Ontology within the nanosafety community

3.3.1 NANoREG

The NANoREG project (partner JRC) developed a large set of Excel (ISA-Tab-Logic) templates and released them under open license at www.nanoreg.eu/media-and-downloads/templates. eNanoMapper collaborated with JRC for over a year before the templates release, evaluating earlier versions and coming to agreement on usage of the templates as the basis for eNanoMapper templates release was achieved. Within WP3 the templates were analysed, fields automatically extracted and cleaned (details in D3.4). The JRC developed the templates with collaboration with FP7 NANoREG project partners (data providers) for the purposes of data entry. Later the NANoREG entry tool (DET by TNO) was based also on these templates. Thus, the template fields provide a large knowledge base of which fields have to be reported in order to a given assay, and which assays are used to measure a particular endpoint.

There are 835 terms in the Oct 2016 version of the templates. (An interactive display of the fields is part of the documentation site reported in D3.4.) After due consideration of the manpower and time available, it was decided that mapping all of the 835 fields to ontology terms would be beyond the resources available in eNanoMapper project and the following strategy was implemented.

The fields for assays (90) and endpoints (30 fields) were automatically mapped to ontology terms by three different methods (NCBO Recommender (Munteanu et al., 2010), Standard Boolean model and TF/IDF similarity (Manning et al., 2008)), The top hits were then summarised and further analysed manually. 49 New terms were then added to the eNanoMapper ontology by reuse of an existing ontology or by manual curation as necessary. These terms are used to annotate NANoREG database entries and templates. The ontology terms are also an essential part of the search application.

3.3.2 NECID

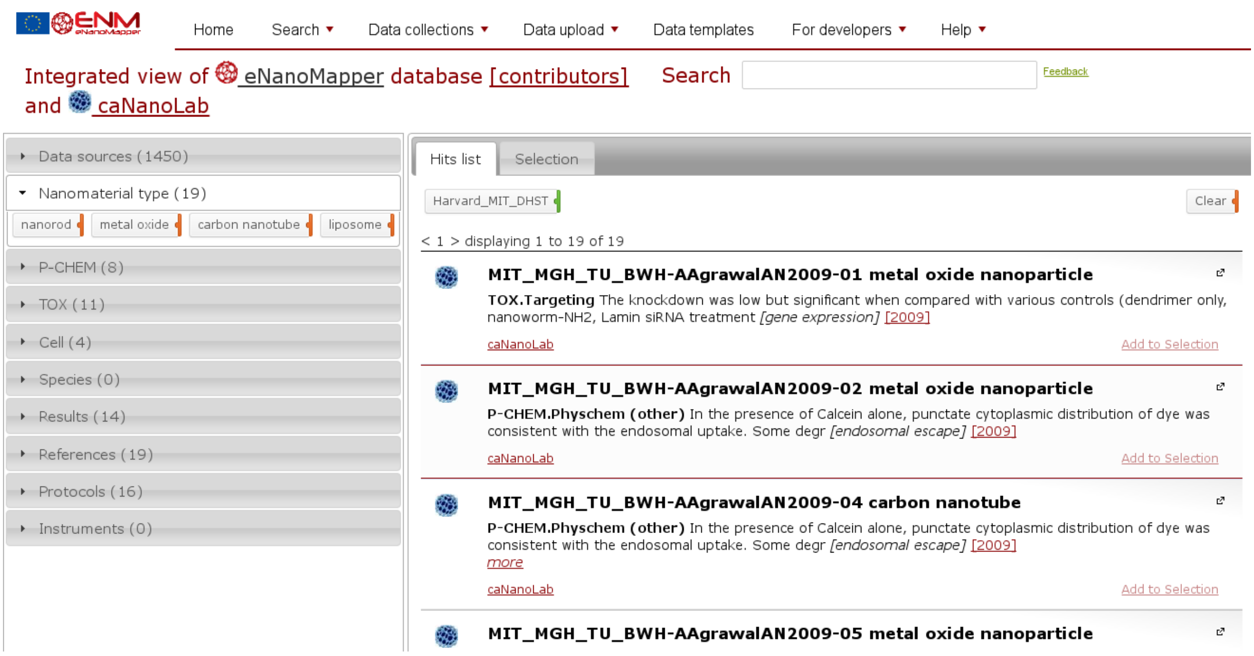
Currently there is an ongoing collaboration between eNM and NECID focussed on mapping database related terms from NECID, concerning occupational exposure assessment, to eNM ontological terms. One of these efforts between these two projects has focussed on mapping OECD nanomaterials. These tasks go hand in hand with connecting the NECID database with the eNM database. As part of this collaboration we have been evaluating of the ontology meets the needs of the content of the NECID database, and in particular the plans to index the content for findability of data in search.data.enanomapper.net. NECID uses the OECD nanomaterials which we have mapped these to ontology IRIs. Because these mappings are expected to be of general interest, we have provided them as guidance online at http://specs.enanomapper.net/oecd/ (see Annex 6.3).

3.3.2 Nanotechnology working group (Nano WG) (Christine Hendren)

As mentioned before, a webinar of the eNM ontology was presented in order to explain the background and the usability to the US-based NanoWG. This webinar, as well as other activities have led to an ongoing collaboration for improving the eNM Ontology and making people in the field more acquainted. Particularly, in the autumn OECD/ProSafe meeting a sketch was made by Nina Jeliazkova (IDEA), Egon Willighagen (UM), and Christine Hendren (NanoWG and others) showing how mutual benefit can be reached around continued development of the ontology and data curation. It should be noted at this point that eNanoMapper co-maintained the NanoParticle Ontology (NPO) and made a number of extensions to the NPO, showing how such collaboration can take place.

3.3.3 caNanolab Data Annotation

Data from the caNanolab was annotation with ontology terms and make searchable in the search.data.enanomapper.net website. The following screenshot shows show data from Boston (Harvard-MIT-DHST filter in green) with nanomaterial type ontology terms (orange tags in the faceted browser on the left):



3.4 Domain coverage of the eNM Ontology within nanosafety field

3.4.1 Modelling and nano-descriptors of nanomaterials

In order to define modeling-related items and functionality, eNanoMapper members from NTUA, EMBL-EBI and UM worked together to compile a list and definitions for a number of ontology terms that needed to be added to the ontology. Work on this was carried out during the weekly meetings, exchange of emails and the Hackathon on Ontology for Modelling & Nano-Descriptors that took place in Athens, Greece on April 11, 2016. This work resulted to adding 162 new terms to the ontology describing experimental and calculated (Image Analysis and algorithm-derived) descriptors, the processes that lead to their generation, modeling, statistics and algorithms. Previous ontologies related to modeling offered only fragmented coverage, with term definitions that were quite often oriented at the specific work or needs of the ontology they were a part of.

3.4.2 Read-across predictions using nano-lazar

The nano-lazar GUI (https://nano-lazar.in-silico.ch) is a graphical frontend for nano-lazar read-across predictions. It makes havy use of eNanoMapper ontologies to explain domain-specific terms (e.g.

various nanoparticle properties) and to provide supplemental information for toxicity predictions. The lazar backend (https://github.com/opentox/lazar) uses ontologies to parse and aggregate eNanoMapper data and to import them into the lazar database backend.

3.5 Definition coverage of the eNM Ontology within nanosafety domain

3.5.1 European Chemicals Agency (ECHA)

On ECHA's request, eNanoMapper presented few solutions which were developed and could be further implemented in the EU observatory of Nanomaterials. The primary goal of the observatory is to provide user friendly and reliable search facilities for wide range of users. The discussion topic most relevant to ontology development was how the enanoMapper ontology relates to the regulatory terminology, such as REACH (the EU regulation concerning the Registration, Evaluation, Authorisation & restriction of CHemicals).

The current status is that eNanoMapper ontology does not directly include definitions of the regulatory terms, but provides a basis to define these by standard ontology constructs as axioms. This approach was selected as the most appropriate, given the evolving nature of the regulatory terminology. Regarding the representation of the experimental data, the enanoMapper ontology includes the REACH endpoints (list of mappings between REACH endpoints and ontology terms in Annex 6.2), extended with large number of new in-vitro endpoints and assays, resulting from NANoREG project, which are expected to be considered for regulatory purposes.

3.5.2 European/JRC definitions

The JRC defined a number of representative industrial nanomaterials for the NanoSafety Cluster to evaluate the physochemical and biological properties of. These materials have identifiers starting with JRCNM and cover various metal oxides (coated and uncoated) and carbon nanotubes. We explored how well our ontology captured these materials and found that all types had similar terms in the ontology. However, for simplicity we ultimately added the specific JRC materials as explicit terms in the ontology, which allows more targeted searches and data integration. These mappings have been made as a guidance available on http://specs.enanomapper.net/jrc/ (see also Annex 6.4).

3.5.3 International Organization for Standardization (ISO) definitions

Because it was considered essential for adoption that the ontology, the project decided to make it openly available. The idea here is that for people to understand the meaning of terms properly they need to have access to the definition and ontological context. Moreover, for the sustainability it is important that people can take the current ontology and continue working on it, which requires an Open Science approach. Being able to extend the ontology is important because we have not been able to cover all research domains that are part of the NSC community. Furthermore, because this research field is a new field, terminology is expected to regularly be updated, something we see for example with the definition of what a nanomaterial is.

However, ISO and OECD standards are commonly not available under an open license, disallowing modification and redistribution. While the legal aspects of this are still being explored, it has not been able for the project, so far, to just copy and paste definitions of terms defined in ISO standards and

OECD reference documents. That does not imply the ontology is not compatible with these standards, but legally it is yet unclear how the two worlds can be merged.

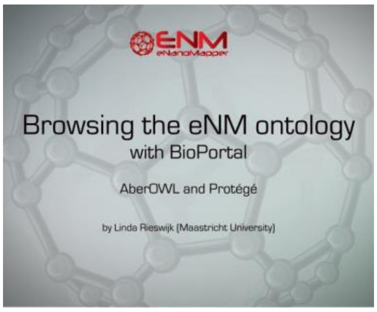
3.6 Collaborations with upstream ontologies

The eNanoMapper ontology reuses several other ontologies, as detailed before. The UM and EMBL-EBI teams have been in contact with several upstream ontologies regarding updates, including NPO, ENVO, BAO, and SIO. Other upstream ontologies actually originate from these two partners, viz. CHEMINF and CHEBI. We have provided feedback to several other ontologies about our needs, though this too is an ongoing process.

3.7 Tutorials

As described in more detail in D6.3 a tutorial was developed for browsing the ontology through online repositories or accessing it locally.

3.7.1 Browsing the eNM Ontology with BioPortal, Aber-OWL and Protégé



http://www.enanomapper.net/library/browsing-ontology

Authors: Linda Rieswijk, Friederike Ehrhart and Egon Willighagen (Maastricht University)

4. CONCLUSION

This deliverable reports on the final release of the ontology during the eNanoMapper project. We have reported on the growth of the ontology and the various internal and external validation processes that led to this growth. Besides specific feedback asked for and given by external expert and other NanoSafety Cluster projects, a few active collaboration with NANoREG, NECID, and others have given of long lists of terms that needed to be covered. We particularly thank those who have shared database schemas and spreadsheet designs with us, allowing us to measure up the completeness of our ontology. We have identified needs that are yet to be implemented, and observed that we have only started to address to full breadth of the field. Yet, with various implementations of use cases we show how useful the current ontology already is, providing faceted searching in the search website (search.data.enanomapper.net), in answering scientific questions using the RDF export of data in combination with the ontology (D3.4), and in supporting data curation (D5.6). The modular approach allowed us to develop an ontology construction pipeline that can be automated and automatically validated for certain requirements (such as the presence of a label and definition). With pleasure we presented this in a final 4.0 release of the ontology, covering various subdomains of the nanosafety domain with no less than 10 thousand terms.

5. BIBLIOGRAPHY

Munteanu, C.R., Pereira, J., Pazos, A., Romero, M.M., & Vázquez-Naya, J.M. (2010). An Approach for the Automatic Recommendation of Ontologies Using Collaborative Knowledge. *KES*. R script for NCBO available on https://github.com/muntisa/RNCBO

Manning, Christopher D., Prabhakar Raghavan, and Hinrich Schütze. Introduction to information retrieval. Vol. 1. No. 1. Cambridge: Cambridge university press, 2008.

6. ANNEXES

ANNEX 6.1 RESULTS OF THE SURVEY ON THE EVALUATION OF THE ENM ONTOLOGY

Timestamp	1. Choose a term which is relevant for your field	2. Please give a brief definition of the term	3. Were you able to find the term?	4. Do you agree with the definition provided within the eNanoMapper ontology?	5. Do the super classes make sense to your field (if applicable)?	6. Do the sub classes make sense to your field (if applicable)?	7. Do you agree with the logical structure leading towards the term of interest?	8. Additional comments
3-3-2016 12:28	information retrieval	fuzzy searching	wikipedia		machine learning	Dirchlet smoothing	yes	
3-3-2016 12:30	SMILES	A line notation that describes (part of) the chemical structure of a nanoparticle.	yes	"SMILES descriptor" captures it, but I would not always use "descriptor" in this context.	yes	yes	yes	this one was too easy.
3-3-2016 12:36	mutagenicity	mutagenicity of a nanoparticle	http://purl.obolibrary.org/obo/MI_2138	it is not in ENM	It does not make sense.	no subclass available	no	
12-4-2016 10:55	Test	Test	Test	Test	Test	Test	Test	Test
12-4-2016 11:57	cytotoxicity	Adverse effects tested on cells	Yes	There is no definition in eNanoMapper but NanoParticle Ontology ontology - I don't agree with the definition	Yes	Not applicable	Yes	
11-10-2016 12:46	Term	Term						
24-10-2016 17:07	High-throughput screening	Screening of several agents for the same endpoint in one test	No					
24-10-2016 17:07	doxirubicin-loaded nanoparticle	Should be under drug-loaded nanoparticle	yes	no definition provided (self explanatory)	No	yes		
24-10-2016 17:11	etoposide-loaded nanoparticle	A drug loaded nanoparticle that is loaded with etoposide	yes	no definition given (self-explanatory)	No	N/A		
24-10-2016 17:11	Environmental Ageing	The transformations (physical, chemical or adsorption of biomolecules) that ENMs undergo upon release into the environment. An example could be sulfidation.	No	No entry so no definition	Partially - Super class would be the class of Ageing or Aged ENM, but needs to be linked to the base ENM, term of interest could be further broken down into the types of environmental ageing, e.g. physical, chemical, biomolecule adsorption.	Yes: sub-class could be the speciation forms (e.g. sulfidated, ionic, particulate, oxidised, soluble and insoluble species forming that depend on media conditions).	Yes but it goes both ways, as can also have precipitation of ENMs from dissolved metals in solution / in vitro / in vivo.	Possiby for full speciation mapping would want % of initial ENM amount, but whether it should be by mass (but not great) or by molar concentration of the different species, which will change over a few seconds / minutes and may then continue to evolve?
24-10-2016 17:11	nanomaterial	Material with size under 100 nm	Yes	Yes.	yes	Yes, but difficult to say if all 'nanomaterials' are listed	Yes	

24-10-2016 17:29	metal nanoparticle	A nanoparticle consisting primarily of a metal	yes	none provided (needs one to differentiate whether only nanoparticles consisting of all metal or mostly metal. Is it based only on core composition?)	should also include inorganic nanoparticle			
24-10-2016 17:30	transcription profiling	Profiling of genome wide gene expression in a biological sample	Yes	Yes, but there is also redundant terms, like gene expression assay	Yes	Yes	Yes	Both transcription profiling assay and gene expression profiling are relevant, but redundant and may cause confusion. Nevertheless, there are non-redundant sub-terms, which makes it difficult to exclude either one.
24-10-2016 17:36	dissolution		yes	definition not available	not really	not applicable	no	from our point of view, the term would better fit into "characterisation"
24-10-2016 17:40	Zeta potential	We need to make more evident the difference among: zeta potential by QM (http://bioportal.bioontology.org/ontologies/ENM/?p=classes&conceptid=http%3A%2F%2Fpurl.enanomapper.org%2Fonto%2FENM_8000111&jump_to_nav=true), zeta potential measured experimentally (http://bioportal.bioontology.org/ontologies/ENM/?p=classes&conceptid=http%3A%2F%2Fpurl.bioontology.org%2Fontology%2Fnpo%23NPO_1302&jump_to_nav	yes		yes			Zeta potential by QM should have different name, such as zeta potential Quantum mechanics calculation
24-10-2016 17:41	Mixture	Mixture is composed of two or more compounds, but not chemically binded.	No	No, I could not find the definition on eNanoMapper	Not enough. Mixtures should cover not only organic materiala but also inorganic ones.	Yes	Yes	Thanks for this great contribution. This would be useful sources to develop models.

Annex 6.2 OECD Harmonised Template Classes to ENM Ontology Mappings

#	Title	I5 Template	Ontology URI	Endpoints	Conditions	Parameters
4.1.	Appearance	GI_GENERAL_INFORM		gaseous, liquid, solid, Not specified	Remark	
4.2.	Melting point / freezing point	PC_MELTING	CHEMINF_000256	Melting Point	Decomposition, Sublimation	
4.3.	Boiling point	PC_BOILING	CHEMINF_000257	Boiling point	Decomposition, Atm. Pressure	
4.5.	Particle size distribution (Granulometry)	PC_GRANULOMETRY	CHMO_0002119	MASS MEDIAN DIAMETER, MASS MEDIAN AERODYNAMIC DIAMETER, GEOMETRIC STANDARD DEVIATION, PARTICLE SIZE	SEQ_NUM, Remark	TESTMAT_FORM, DISTRIBUTION_TYPE
4.6.	Vapour pressure	PC_VAPOUR	CHEMINF_000419			
4.7.	Partition coefficient	PC_PARTITION	BAO_0002130	Vapour Pressure	Temperature	
4.8.	Water solubility	PC_WATER_SOL	BAO_0002775	Water solubility	Temperature	Method type
4.9.	Solubility in organic solvents	PC_SOL_ORGANIC	BAO_0002135	Solubility org. solvents	Temperature, Remark, Solvent	
4.20.	pH	PC_NON_SATURATED_PH	UO_0000196	pH	Temperature, Doses/concentrations, Remark	
4.21.	Dissociation constant	PC_DISSOCIATION	CHEMINF_000194	pKa	Temperature, No.	
4.24.	Agglomeration/aggregation	AGGLOMERATION_AGGREGATION	NPO_1967 NPO_1968	AGGLO_AGGR_DIAM, AGGLO_AGGR_SIZE, AGGLO_AGGR_SIZE_DIST, AGGLO_AGGREGATION_IDX	pH, MEDIUM, Remark, SEQ_NUM, PHRASEOTHER_PERCENTILE	Method details, DATA_GATHERING_INSTRUMENTS, SAMPLING, Type of method
4.25.	Crystalline phase	CRYSTALLINE_PHASE	NPO_1512	CRYSTALLINE PHASE		Method details, DATA_GATHERING_INSTRUMENTS, SAMPLING, Type of method, TESTMAT_FORM, MATERIAL_ISOTROPIC
4.26.	Crystallite and grain phase	CRYSTALLITE_AND_GRAIN_SIZE		MEAN DIAMETER		Method details, DATA_GATHERING_INSTRUMENTS, SAMPLING, Type of method, TESTMAT_FORM, MATERIAL_ISOTROPIC
4.27.	Aspect ratio/shape	ASPECT_RATIO_SHAPE	NPO_274 NPO_1365	X, Y, Z, SHAPE	Remark	Method details, DATA_GATHERING_INSTRUMENTS, SAMPLING, Type of method
4.28.	Specific surface area	SPECIFIC_SURFACE_AREA	NPO_1235	SPECIFIC_SURFACE_AREA	Remark	Method details, DATA_GATHERING_INSTRUMENTS, SAMPLING, TESTMAT_FORM, Type of method
4.29.	Zeta potential	ZETA_POTENTIAL	NPO_1302	ZETA POTENTIAL, ISOELECTRIC POINT	MEDIUM, pH, Remark	Method details, DATA_GATHERING_INSTRUMENTS, SAMPLING, TESTMAT_FORM, Type of method

4.30.	Surface chemistry	SURFACE_CHEMISTRY		ATOMIC COMPOSITION, FUNCTIONAL GROUP	COATING_DESCRIPTION, DESCRIPTION, Remark, ELEMENT_OR_GROUP, TYPE	Method details, DATA_GATHERING_INSTRUMENTS, SAMPLING, Type of method

4.31.	Dustiness	DUSTINESS	ENM_9000003	DUSTINESS INDEX		Method details, DATA_GATHERING_INSTRUMENTS, SAMPLING, Type of method, TESTMAT_FORM
4.32.	Porosity	POROSITY	PATO_0000973	POROSITY, SPECIFIC PORE VOLUME		Method details, DATA_GATHERING_INSTRUMENTS, SAMPLING, Type of method, TESTMAT_FORM
4.33.	Nanomaterial pour density	POUR_DENSITY	ENM_9000004	POUR DENSITY		Method details, DATA_GATHERING_INSTRUMENTS, SAMPLING, Type of method, TESTMAT_FORM
4.34.	Nanomaterial photocatalytic activity	PHOTOCATALYTIC_ACTIVITY		PHOTOCATALYTIC ACTIVITY, TURN OVER FREQUENCY		Method details, DATA_GATHERING_INSTRUMENTS, SAMPLING, Type of method, TESTMAT_FORM
4.36.	Nanomaterial catalytic activity	CATALYTIC_ACTIVITY		CATALYTIC ACTIVITY, TURN OVER FREQUENCY		Method details, DATA_GATHERING_INSTRUMENTS, SAMPLING, Type of method, TESTMAT_FORM
4.99.	PC UNKNOWN	Physico chemical properties (other)				
5.1.1.	Phototransformation in Air	TO_PHOTOTRANS_AIR		DT50	Reactant, Test condition	Reactant
5.1.2.	Hydrolysis	TO_HYDROLYSIS			pH, Temperature	
5.2.1.	Biodegradation in water - screening tests	TO_BIODEG_WATER_SCREEN		% Degradation, CH4 evolution, CO2 evolution, DOC removal, inorg. C analysis, O2 consumption, Radiochem. meas., Test mat. analysis, TOC removal	Sampling time	Test type
5.2.2.	Biodegradation in water and sediment: simulation tests	TO_BIODEG_WATER_SIM		(pseudo-)first order (= DT50), second order, zero order	Test type, Degradation Parameter, Degradation, Sampling time	Test type
5.2.3.	Biodegradation in Soil	EN_STABILITY_IN_SOIL		(pseudo-)first order (= DT50), second order, zero order, other:, no data	Test type, Soil No., Soil type, OC content	Test type
5.3.1.	Bioaccumulation: aquatic / sediment	EN_BIOACCUMULATION		BCF, BAF, BSAF, BMF	Route, Bioacc. basis, Doses/concentrations	Species, Route
5.3.2.	Bioaccumulation: terrestrial	EN_BIOACCU_TERR		BCF, BSAF	Bioacc. basis	Species
5.4.1.	Adsorption / Desorption	EN_ADSORPTION		Koc, log Koc, Kd, other:	Temperature, % Org.Carbon, Remark	
5.4.2.	Henry's Law constant	EN_HENRY_LAW	CHEMINF_000433	Henry's Law const.	Pressure, Temperature, Remark	
6.1.1.	Short-term toxicity to fish	EC_FISHTOX	ENM_0000010	LC0, LC10, LC50, LC100, EC0, EC10, EC50, EC100, LL0, LL10, LL50, LL100, EL0, EL10, EL50, EL100, IC10, IC50, IC100, NOELR, LOELR, NOEC, LOEC	Effect, Based on, Measured concentration, Exposure	Exposure, Test Medium, Test organism

6.1.2.	Long-term toxicity to fish	EC_CHRONFISHTOX	ENM_0000011	NOEC, LOEC, NOELR, LOELR, EC10, EC50, EL10, EL50, IC10, IC50, LC10, LC50, LL10, LL50	Effect, Based on, Measured concentration, Exposure	Exposure, Test Medium, Test organism

6.1.4.	Long-term toxicity to aquatic inverterbrates	EC_CHRONDAPHNIATOX		NOEC, LOEC, NOELR, LOELR, EC10, EC50, EL10, EL50, IC10, IC50, LC10, LC50, LL10, LL50	Effect, Based on, Measured concentration, Exposure	Exposure, Test Medium, Test organism
6.1.5.	Toxicity to aquatic algae and cyanobacteria	EC_ALGAETOX	ENM_0000005	EC0, EC5, EC10, EC20, EC50, EC90, EC100, EL0, EL5, EL10, EL20, EL50, EL90, EL100, IC10, IC50, IC100, NOEC, NOELR, LOEC, LOELR	Effect, Based on, Measured concentration, Exposure	Exposure, Test Medium, Test organism
6.1.7.	Toxicity to microorganisms	EC_BACTOX	ENM_0000015	EC0, EC10, EC50, EC100, IC0, IC10, IC50, IC100, NOEC, LOEC	Effect, Based on, Measured concentration, Exposure	Exposure, Test Medium, Test organism
6.2.	Sediment toxicity	EC_SEDIMENTDWELLING TOX	ENM_0000009	LC0, LC10, LC50, LC100, EC0, EC10, EC50, EC100, LD0, LD10, LD50, LD100, LR0, LR10, LR50, LR100, NOEC, LOEC, other:	Based on, Exposure, Measured concentration, Effect	Test Medium, Test organism, Exposure
6.3.1.	Toxicity to soil macroorganisms	EC_SOILDWELLINGTOX	ENM_0000013	LC0, LC10, LC50, LC100, EC0, EC10, EC50, EC100, LD0, LD10, LD50, LD100, LR0, LR10, LR50, LR100, NOEC, LOEC, other:	Based on, Exposure, Measured concentration, Effect	Test Medium, Test organism, Exposure
6.3.2.	Toxicity to terrestrial arthropods	EC_HONEYBEESTOX	ENM_0000016	LC0, LC10, LC50, LC100, EC0, EC10, EC50, EC100, LD0, LD10, LD50, LD100, LR0, LR10, LR50, LR100, NOEC, LOEC, other:	Based on, Exposure, Measured concentration, Effect	Test organism, Exposure
6.3.3.	Toxicity to terrestrial plants	EC_PLANTTOX	ENM_0000017	NOEC, LOEC, EC0, EC10, EC25, EC50, EC100, ER0, ER10, ER25, ER50, ER100, LC0, LC10, LC25, LC50, LC100	Test organism, Based on, Exposure, Measured concentration, Effect	Test Medium, Exposure
6.3.4.	Toxicity to soil microorganisms	EC_SOIL_MICRO_TOX	ENM_0000008	EC0, EC10, EC25, EC50, EC100, ER0, ER10, ER25, ER50, ER100, NOEC, other:	Based on, Exposure, Measured concentration, Effect	Test organism, Exposure
7.2.1.	Acute toxicity - oral	TO_ACUTE_ORAL	ENM_0000020	LD0, LD50, LD100, LDLo, approx. LD50, discriminating dose	Species, Sex	
7.2.2.	Acute toxicity - inhalation	TO_ACUTE_INHAL	ENM_0000023	LC0, LC50, LC100, LCLo, discriminating conc.	Species, Sex	
7.2.3.	Acute toxicity - dermal	TO_ACUTE_DERMAL	ENM_0000026	LD0, LD50, LD100, LDLo, approx. LD50, discriminating dose	Species, Sex	
7.3.1.	Skin irritation / Corrosion	TO_SKIN_IRRITATION	ENM_0000032			Species, Type of method
7.3.2.	Eye irritation	TO_EYE_IRRITATION	ENM_0000033			Species, Type of method
7.4.1.	Skin sensitisation	TO_SENSITIZATION	ENM_0000034			Species, Type of method, Type of study
7.5.1.	Repeated dose toxicity - oral	TO_REPEATED_ORAL	ENM_0000021	NOAEL, NOEL, LOAEL, LOEL, BMD05, BMDL05, BMDL10, BMD, BMC05, BMCL05, BMCL10, BMC, dose level, conc. level, other:	Species, Test type, Sex	Route of administration, Doses/concentrations
7.5.2.	Repeated dose toxicity - inhalation	TO_REPEATED_INHAL	ENM_0000024	NOAEL, NOEL, LOAEL, LOEL, BMD05, BMDL05, BMDL10, BMD, BMC05, BMCL05, BMCL10, BMC, dose level, conc. level, other:	Species, Test type, Sex	Route of administration, Doses/concentrations
7.5.3.	Repeated dose toxicity - dermal	TO_REPEATED_DERMAL	ENM_0000027	NOAEL, NOEL, LOAEL, LOEL, BMD05, BMDL05, BMDL10, BMD, BMC05, BMCL05,	Species, Test type, Sex	TYPE_COVERAGE, Doses/concentrations

				BMCL10, BMC, dose level, conc. level, other:		
7.6.1.	Genetic toxicity in vitro	TO_GENETIC_IN_VITRO	http://www.bioassayontology.org/bao#BAO_0002167	GENOTOXICITY	Type of study, Metabolic activation, Species	Type of study, Metabolic activation system, Type of genotoxicity, Target gene, Species
7.6.2.	Genetic toxicity in vivo	TO_GENETIC_IN_VIVO	ENM_0000028	GENOTOXICITY	Type of study, Toxicity, Sex	Route of administration, Type of study, Type of genotoxicity, Species
7.7.	Carcinogenicity	TO_CARCINOGENICITY	ENM_0000029	no NOAEC identified, no NOAEL identified, no T25 identified, T25, NOAEC, NOAEL, NOEC, NOEL, LOAEC, LOAEL, LOEC, LOEL, BMD05, BMDL05, BMDL10, BMD, BMC05, BMCL05, BMCL10, BMC, dose level, conc.level, other:	Species, Effect type	Species, Route of administration, Doses/concentrations
7.8.1.	Toxicity to reproduction	TO_REPRODUCTION		NOAEL, NOEL, LOAEL, LOEL, BMD05, BMDL05, BMDL10, BMD, BMC05, BMCL05, BMCL10, BMC, dose level, conc. level, other:	Species, Sex, Generation	Species, Route of administration, Doses/concentrations
7.8.2.	Developmental toxicity / teratogenicity	TO_DEVELOPMENTAL		NOAEL, NOEL, LOAEL, LOEL, BMD05, BMDL05, BMDL10, BMD, BMC05, BMCL05, BMCL10, BMC, dose level, conc. level, other:	Species, Effect type	Species, Route of administration, Doses/concentrations

Annex 6.3 Mappings to the eNanoMapper ontology for the OECD nanomaterials

Annex 6.4 Mappings to the eNanoMapper ontology for the JRC nanomaterials

eNanoMapper Ontology IRIs for the OECD nanomaterials

eNanoMapper Working Draft 26 November 2016

This version:
: http://specs.enanomapper.org/2016/WD-oecd-20161126/

Latest published version:
: http://specs.enanomapper.org/oecd/

Previous version:
: none

Editor:
: Egon Willighagen, Maastricht University

Abstract

The OECD has a list of nanomaterials of interest. eNanoMapper is developing an ontology to be used as common language by this community. This document links the OECD materials to specific terms in the ontology and provides identifiers for each of them.

Status of This Document

This document is a specification by eNanoMapper. It has no official standing of any kind and does not represent the support or consensus of any standards organisation.

Intended audience

This document is aimed at everyone working in the NanoSafety Cluster.

Table of Contents

1. Introduction

This section is non-normative.

The eNanoMapper ontology is developed to be used as common language for the nanosafety community [*Hastings2015*]. The ontology contains terms for, for example, titanium dioxide and zinc oxide, but the encourage the data and knowledge exchange for the OECD nanomaterials, we have added them to the ontology specifically.

2. The mappings

The below table gives the ontology IRIs for each of the JRC representative nanomaterials. The links provided for the ontology IRIs point to BioPortal [*Noy2009*]. Clear from the mappings is how the eNanoMapper ontology [*Hastings2015*] builds on the efforts from the NanoParticle Ontology [*Thomas2011*] and ChEBI ontology [*Hastings2012*].

OECD nanomaterial	Code	Full Ontology IRI
cerium oxide nanoparticles	ENM_9000006	http://purl.enanomapper.org/onto/ENM_9000006
multi-walled carbon nanotubes	NPO_354	http://purl.bioontology.org/ontology/npo#NPO_354
single-walled carbon nanotubes	NPO_943	http://purl.bioontology.org/ontology/npo#NPO_943
dendrimers	NPO_735	http://purl.bioontology.org/ontology/npo#NPO_735
nanoclay nanoparticles	ENM_9000007	http://purl.enanomapper.org/onto/ENM_9000007
titanium dioxide nanoparticles	CHEBI_51050	http://purl.obolibrary.org/obo/CHEBI_51050
fullerenes	CHEBI_33128	http://purl.obolibrary.org/obo/CHEBI_33128
silicon dioxide nanoparticles	CHEBI_33128	http://purl.obolibrary.org/obo/CHEBI_33128
zinc oxide nanoparticles	NPO_1542	http://purl.bioontology.org/ontology/npo#NPO_1542
gold nanoparticles	NPO_401	http://purl.bioontology.org/ontology/npo#NPO_401
silver nanoparticles	NPO_1892	http://purl.bioontology.org/ontology/npo#NPO_1892
iron nanoparticles	ENM_9000200	http://purl.enanomapper.org/onto/ENM_9000200
aluminium oxide nanoparticles	ENM_9000005	http://purl.enanomapper.org/onto/ENM_9000005

A. References

A.1 Normative references

No normative references.

A.2 Informative references

[Hastings2012]

Hastings, J., de Matos, P., Dekker, A., Ennis, M., Harsha, B., Kale, N., Muthukrishnan, V., Owen, G., Turner, S., Williams, M., Steinbeck, C., Nov. 2012. The ChEBI reference database and ontology for biologically relevant chemistry: enhancements for 2013. Nucleic Acids Research 41 (D1), D456-D463. http://dx.doi.org/10.1093/nar/gks1146

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Hastings, J., Jeliazkova, N., Owen, G., Tsiliki, G., Munteanu, C. R., Steinbeck, C., Willighagen, E., Mar. 2015. eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment. Journal of Biomedical Semantics 6 (1), 10+, http://dx.doi.org/10.1186/s13326-015-0005-5.

[Noy2009]

Noy, N. F., Shah, N. H., Whetzel, P. L., Dai, B., Dorf, M., Griffith, N., Jonquet, C., Rubin, D. L., Storey, M. A., Chute, C. G., Musen, M. A., May 2009. BioPortal: ontologies and integrated data resources at the click of a mouse. Nucleic Acids Research 37 (Web Server), W170-W173, http://dx.doi.org/10.1093/nar/gkp440.

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Thomas, D. G., Pappu, R. V., Baker, N. A., Feb. 2011. NanoParticle ontology for cancer nanotechnology research. Journal of Biomedical Informatics 44 (1), 59-74. http://dx.doi.org/10.1016/j.jbi.2010.03.001

eNanoMapper Ontology IRIs for the JRC representative industrial nanomaterials

eNanoMapper Working Draft 16 January 2017

This version:
http://specs.enanomapper.org/2017/WD-template-20170116/
Latest published version:
http://specs.enanomapper.org/template/
Previous version:
none
Editor:
Egon Willighagen, Maastricht University
Author:
Jiakang Chang, EMBL-EBI

Abstract

The JRC representative industrial nanomaterials are a series of nanomaterials used in the European nanosafety community for research. eNanoMapper is developing an ontology to be used as common language by this community. This document links the JRC materials to specific terms in the ontology and provides identifiers for each of them.

Status of This Document

This document is a specification by eNanoMapper. It has no official standing of any kind and does not represent the support or consensus of any standards organisation.

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2. The mappings

The below table gives the ontology IRIs for each of the JRC representative nanomaterials. The links provided for the ontology IRIs point to BioPortal [*Noy2009*].

JRC nanomaterial	Code	Ontology IRI	Wikidata
JRCNM01000a	ENM_9000074	http://purl.enanomapper.org/onto/ENM_9000074	Q27918612
JRCNM01001a	ENM_9000075	http://purl.enanomapper.org/onto/ENM_9000075	
JRCNM01002a	ENM_9000076	http://purl.enanomapper.org/onto/ENM_9000076	
JRCNM01003a	ENM_9000083	http://purl.enanomapper.org/onto/ENM_9000083	
JRCNM01004a	ENM_9000084	http://purl.enanomapper.org/onto/ENM_9000084	
JRCNM01005a	ENM_9000077	http://purl.enanomapper.org/onto/ENM_9000077	
JRCNM01100a	ENM_9000078	http://purl.enanomapper.org/onto/ENM_9000078	
JRCNM01101a	ENM_9000086	http://purl.enanomapper.org/onto/ENM_9000086	
JRCNM02000a	ENM_9000087	http://purl.enanomapper.org/onto/ENM_9000087	
JRCNM02001a	ENM_9000088	http://purl.enanomapper.org/onto/ENM_9000088	
JRCNM02002a	ENM_9000089	http://purl.enanomapper.org/onto/ENM_9000089	
JRCNM02003a	ENM_9000090	http://purl.enanomapper.org/onto/ENM_9000090	
JRCNM02004a	ENM_9000091	http://purl.enanomapper.org/onto/ENM_9000091	
JRCNM02004b	ENM_9000092	http://purl.enanomapper.org/onto/ENM_9000092	
JRCNM03300a	ENM_9000097	http://purl.enanomapper.org/onto/ENM_9000097	
JRCNM03301a	ENM_9000098	http://purl.enanomapper.org/onto/ENM_9000098	
JRCNM04000a	ENM_9000080	http://purl.enanomapper.org/onto/ENM_9000080	
JRCNM04001a	ENM_9000081	http://purl.enanomapper.org/onto/ENM_9000081	
JRCNM10201a	ENM_9000094	http://purl.enanomapper.org/onto/ENM_9000094	
JRCNM10404	ENM_9000093	http://purl.enanomapper.org/onto/ENM_9000093	
JRCNM62001a	ENM_9000095	http://purl.enanomapper.org/onto/ENM_9000095	
JRCNM62002a	ENM_9000096	http://purl.enanomapper.org/onto/ENM_9000096	
JRCNM62101a	ENM_9000079	http://purl.enanomapper.org/onto/ENM_9000079	

A. References

A.1 Normative references

No normative references.

A.2 Informative references

[Hastings2015]

Hastings, J., Jeliazkova, N., Owen, G., Tsiliki, G., Munteanu, C. R., Steinbeck, C., Willighagen, E., Mar. 2015. eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment. Journal of Biomedical Semantics 6 (1), 10+, http://dx.doi.org/10.1186/s13326-015-0005-5.

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Noy, N. F., Shah, N. H., Whetzel, P. L., Dai, B., Dorf, M., Griffith, N., Jonquet, C., Rubin, D. L., Storey, M. A., Chute, C. G., Musen, M. A., May 2009. BioPortal: ontologies and integrated data resources at the click of a mouse. Nucleic Acids Research 37 (Web Server), W170-W173, http://dx.doi.org/10.1093/nar/gkp440.