

# Ontologies to support FAIR research output

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*Nanosafety and the semantic web: from natural language  
to computational processing*

Zoom, 2021-12-8/9

# Common solutions for the community

NanoReg<sup>2</sup>



OpenRiskNet



# The eNanoMapper Ontology (some history)

Hastings et al. *Journal of Biomedical Semantics* (2015) 6:10  
DOI 10.1186/s13326-015-0005-5



BEILSTEIN JOURNAL OF NANOTECHNOLOGY

## RESEARCH

## Open Access

## eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment

Janna Hastings<sup>1\*</sup>, Nina Jeliaskova<sup>2</sup>, Gareth Owen<sup>1</sup>, Georgia Tsiliki<sup>3</sup>, Cristian R Munteanu<sup>4,5</sup>, Christoph Steinbeck<sup>1</sup> and Egon Willighagen<sup>5</sup>

### Abstract

Engineered nanomaterials (ENMs) are being developed to meet specific application needs in diverse domains across the engineering and biomedical sciences (e.g. drug delivery). However, accompanying the exciting proliferation of novel nanomaterials is a challenging race to understand and predict their possibly detrimental effects on human health and the environment. The eNanoMapper project ([www.enanomapper.net](http://www.enanomapper.net)) is creating a pan-European computational infrastructure for toxicological data management for ENMs, based on semantic web standards and ontologies. Here, we describe the development of the eNanoMapper ontology based on adopting and extending existing ontologies of relevance for the nanosafety domain. The resulting eNanoMapper ontology is available at <http://purl.enanomapper.net/onto/enanomapper.owl>. We aim to make the re-use of external ontology content seamless and thus we have developed a library to automate the extraction of subsets of ontology content and the assembly of the subsets into an integrated whole. The library is available (open source) at <http://github.com/enanomapper/slimmer/>. Finally, we give a comprehensive survey of the domain content and identify gap areas. ENM safety is at the boundary between engineering and the life sciences, and at the boundary between molecular granularity and bulk granularity. This creates challenges for the definition of key entities in the domain, which we also discuss.

**Keywords:** Nanomaterial, Safety, Ontology

### Background

Nanomaterials are materials in which the individual components are sized roughly in the 1–100 nanometer range.

Counterbalancing the many possible benefits of developed nanotechnology, nanoparticles also pose serious risks to human and environmental health [1]. Recognising

## The eNanoMapper database for nanomaterial safety information

Nina Jeliaskova<sup>\*1</sup>, Charalampos Chomenidis<sup>2</sup>, Philip Doganis<sup>2</sup>, Bengt Fadeel<sup>3</sup>, Roland Grafström<sup>3</sup>, Barry Hardy<sup>4</sup>, Janna Hastings<sup>5</sup>, Markus Hegi<sup>4</sup>, Vedrin Jeliaskov<sup>1</sup>, Nikolay Kochev<sup>1,6</sup>, Pekka Kohonen<sup>3</sup>, Cristian R. Munteanu<sup>7,8</sup>, Haralambos Sarimveis<sup>2</sup>, Bart Smeets<sup>7</sup>, Pantelis Sopasakis<sup>2,9</sup>, Georgia Tsiliki<sup>2</sup>, David Vorgrimmler<sup>10</sup> and Egon Willighagen<sup>7</sup>

### Full Research Paper

### Open Access

#### Address:

<sup>1</sup>Ideaconsult Ltd., Sofia, Bulgaria, <sup>2</sup>National Technical University of Athens, School of Chemical Engineering, Athens, Greece, <sup>3</sup>Karolinska Institutet, Stockholm, Sweden, <sup>4</sup>Douglas Connect GmbH, Zeiningen, Switzerland, <sup>5</sup>European Molecular Biology Laboratory – European Bioinformatics Institute (EMBL-EBI), Hinxton, United Kingdom, <sup>6</sup>Department of Analytical Chemistry and Computer Chemistry, University of Plovdiv, Plovdiv, Bulgaria, <sup>7</sup>Department of Bioinformatics, NUTRIM, Maastricht University, Maastricht, The Netherlands, <sup>8</sup>Computer Science Faculty, University of A Coruña, A Coruña, Spain, <sup>9</sup>IMT Institute for Advanced Studies Lucca, Lucca, Italy and <sup>10</sup>in silico toxicology GmbH (IST), Basel, Switzerland

*Beilstein J. Nanotechnol.* 2015, 6, 1609–1634.  
doi:10.3762/bjnano.6.165

Received: 31 March 2015  
Accepted: 03 July 2015  
Published: 27 July 2015

This article is part of the Thematic Series "Nanoinformatics for environmental health and biomedicine".

Guest Editor: R. Liu

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## Release 7 of the eNanoMapper ontology

laurent2207 released this 22 days ago · [24 commits](#) to master since this release

Version 7 of the eNanoMapper Ontology (ENM) was released on the 4th February 2021.

### What's new in version 7

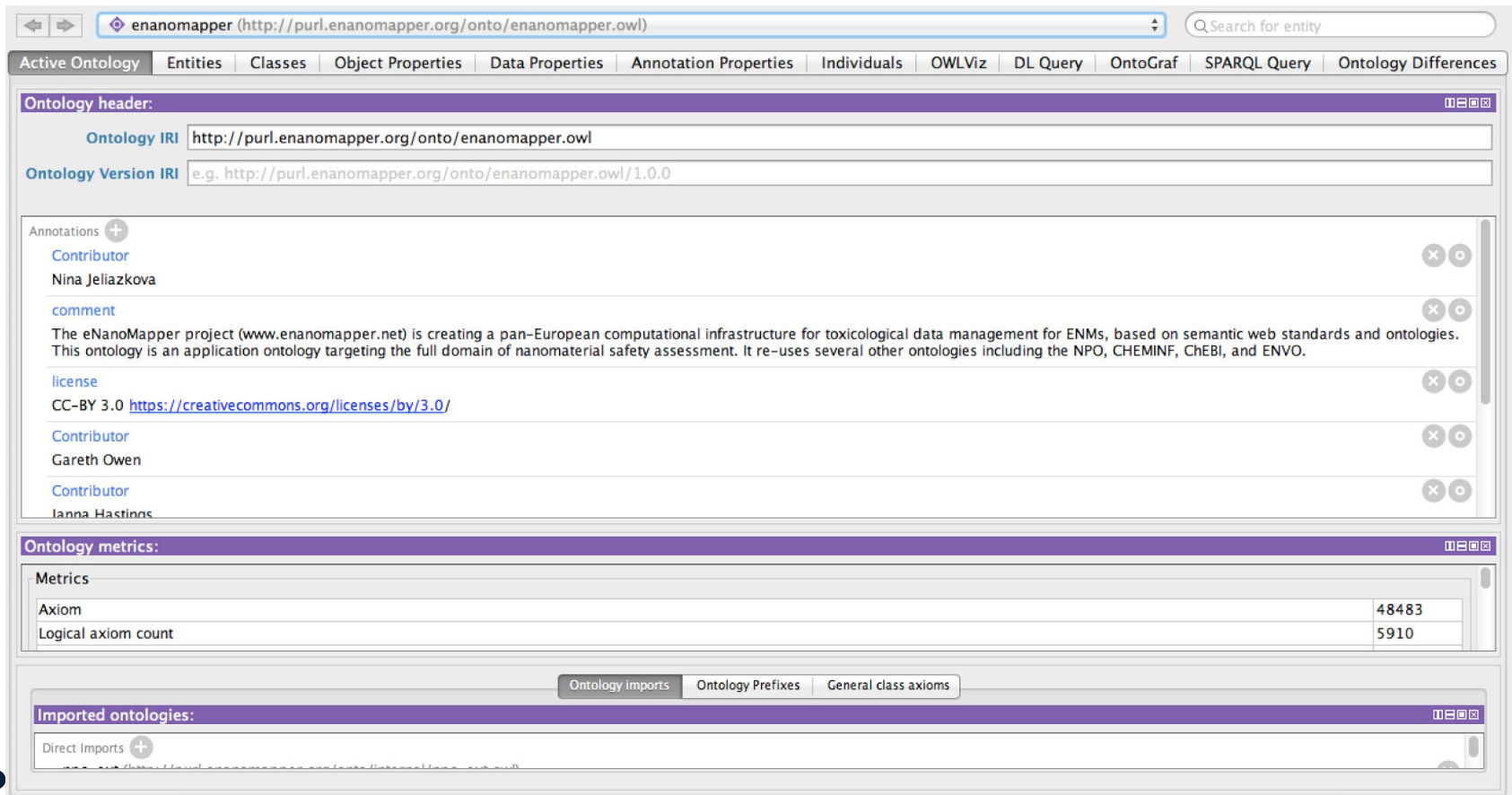
- Addition of properties from various ontologies, such as BAO, CHEMINF, NPO, RO and SIO (see also GitHub issue [#240](#)).
- ACEnano - Analytical and Characterisation Excellence in nanomaterial risk assessment: A tiered approach (Grant Agreement 720952)
- Addition of more JRC materials, for more details see <https://nanocommons.github.io/specifications/jrc/>.
- Updated the GitHub repository with more granular permissions for easier community development.
- Removal of HUPSON slimmed ontology files as we used only one term.
- Integration of MESOCOSM [1] terms by NanoinformaTIX team.

1. A. Ayadi et al. MESOCOSM: A mesocosm database management system for environmental nanosafety. NanoImpact, January(21) 2021. <https://doi.org/10.1016/j.impact.2020.100288>

This release was made by the NanoCommons project which has received funding from European Union Horizon 2020 Programme (H2020) under grant agreement n° 731032. Full funding information is available at <https://github.com/enanomapper/ontologies/blob/master/README.md>

# Download the ontology .owl

Open in Protégé [enanomapper.github.io/onto/enanomapper.owl](http://purl.enanomapper.org/onto/enanomapper.owl)



The screenshot shows a web browser displaying the enanomapper ontology page. The address bar shows the URL <http://purl.enanomapper.org/onto/enanomapper.owl>. The page has a navigation bar with tabs: Active Ontology, Entities, Classes, Object Properties, Data Properties, Annotation Properties, Individuals, OWLViz, DL Query, OntoGraf, SPARQL Query, and Ontology Differences. The main content area is divided into several sections:


- Ontology header:** Contains the Ontology IRI (<http://purl.enanomapper.org/onto/enanomapper.owl>) and the Ontology Version IRI (e.g. <http://purl.enanomapper.org/onto/enanomapper.owl/1.0.0>).
- Annotations:** A list of annotations with expand/collapse icons. The first annotation is for the property `Contributor` with the value `Nina Jeliazkova`. The second annotation is for the property `comment` with the value: "The eNanoMapper project ([www.enanomapper.net](http://www.enanomapper.net)) is creating a pan-European computational infrastructure for toxicological data management for ENMs, based on semantic web standards and ontologies. This ontology is an application ontology targeting the full domain of nanomaterial safety assessment. It re-uses several other ontologies including the NPO, CHEMINF, ChEBI, and ENVO." The third annotation is for the property `license` with the value: "CC-BY 3.0 <https://creativecommons.org/licenses/by/3.0/>". The fourth annotation is for the property `Contributor` with the value `Gareth Owen`. The fifth annotation is for the property `Contributor` with the value `Janna Hastings`.
- Ontology metrics:** A table showing metrics for the ontology.

Metrics	
Axiom	48483
Logical axiom count	5910

Below the metrics table, there are tabs for **Ontology imports**, **Ontology Prefixes**, and **General class axioms**. The **Imported ontologies:** section shows a list of imported ontologies.



# Download and explore on Bioportal

 BioPortal

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## eNanoMapper

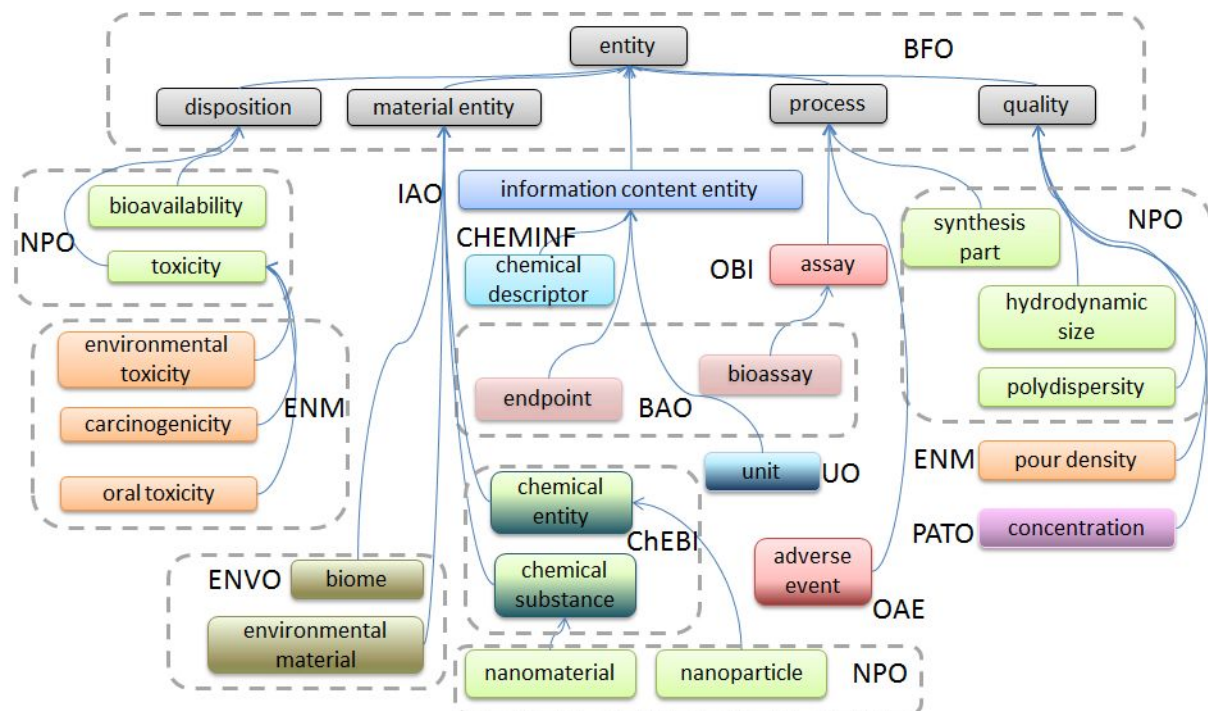
[Summary](#) [Classes](#) [Properties](#) [Notes](#) [Mappings](#) [Widgets](#)

### Details

ACRONYM	ENM
VISIBILITY	Public
BIOPORTAL PURL	<a href="http://purl.bioontology.org/ontology/ENM">http://purl.bioontology.org/ontology/ENM</a>
DESCRIPTION	The eNanoMapper ontology covers the full scope of terminology needed to support research into nanomaterial safety. It builds on multiple pre-existing external ontologies such as the NanoParticle Ontology.
STATUS	Alpha
FORMAT	OWL
CONTACT	Egon Willighagen, <a href="mailto:egon.willighagen@maastrichtuniversity.nl">egon.willighagen@maastrichtuniversity.nl</a> Janna Hastings, <a href="mailto:hastings@ebi.ac.uk">hastings@ebi.ac.uk</a>
HOME PAGE	<a href="https://github.com/enanomapper/ontologies">https://github.com/enanomapper/ontologies</a>
PUBLICATIONS PAGE	
DOCUMENTATION PAGE	
CATEGORIES	Health
GROUPS	

# What's in the ontology?

# The eNanoMapper ontology



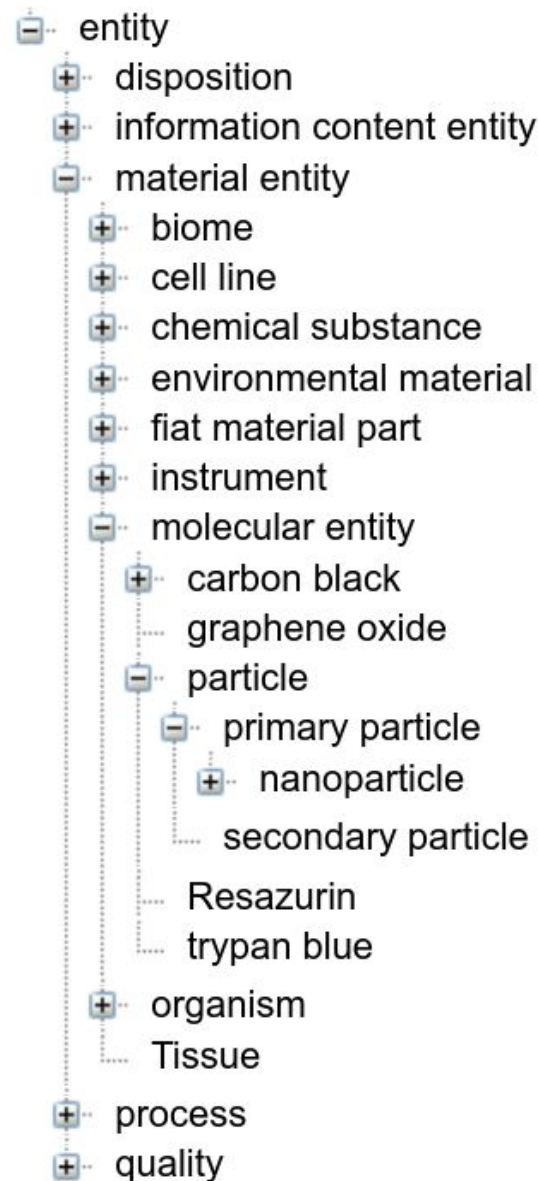
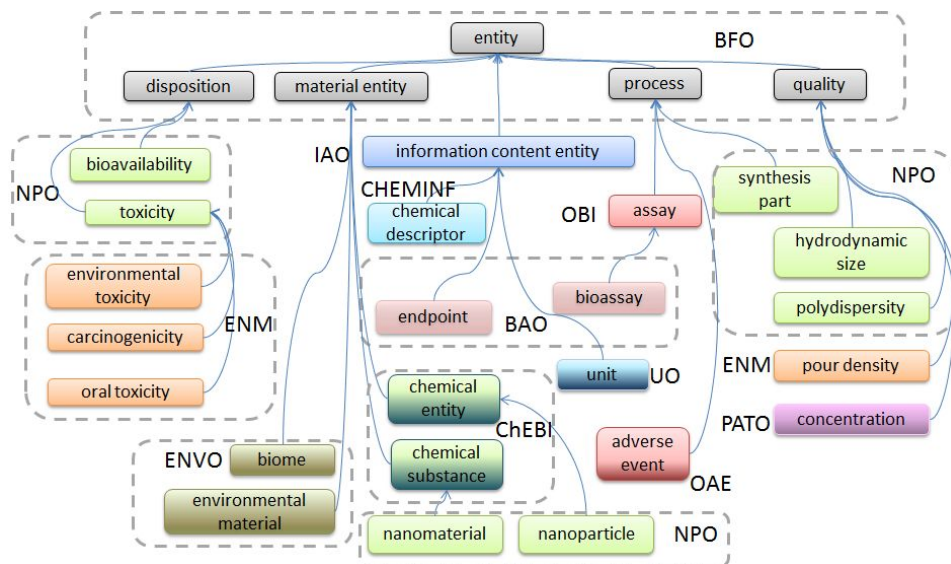
Hastings, J.; Jeliaskova, N.; Owen, G.; Tsiliki, G.; Munteanu, C. R.; Steinbeck, C.; Willighagen, E. eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment. *J. Biomed. Semantics* 2015, 6, 10 DOI: [10.1186/s13326-015-0005-5](https://doi.org/10.1186/s13326-015-0005-5).

N. Jeliaskova et al., The eNanoMapper database for nanomaterial safety information, *Beilstein J. Nanotechnol.*, vol. 6, pp. 1609–1634, Jul. 2015. [10.3762/bjnano.6.165](https://doi.org/10.3762/bjnano.6.165)





# The eNanoMapper ontology



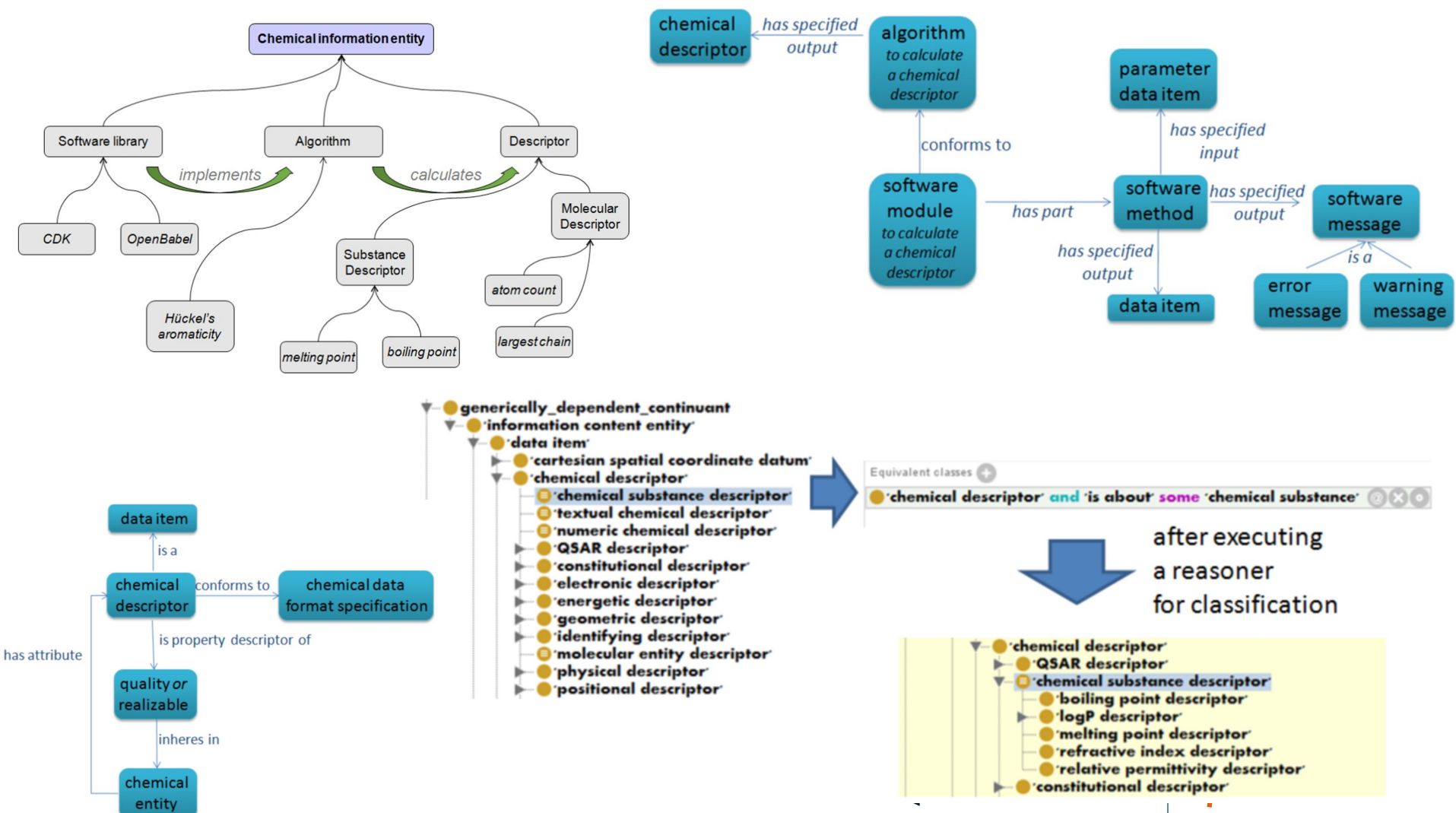
Hastings, J.; Jeliaskova, N.;  
 Owen, G.; Tsiliki, G.; Munteanu,  
 C. R.; Steinbeck, C.; Willighagen,  
 E. eNanoMapper: harnessing  
 ontologies to enable data  
 integration for nanomaterial  
 risk assessment. J. Biomed.  
 Semantics 2015, 6, 10 DOI:  
[10.1186/s13326-015-0005-5](https://doi.org/10.1186/s13326-015-0005-5).

# The Chemical Information Ontology: Provenance and Disambiguation for Chemical Data on the Biological Semantic Web

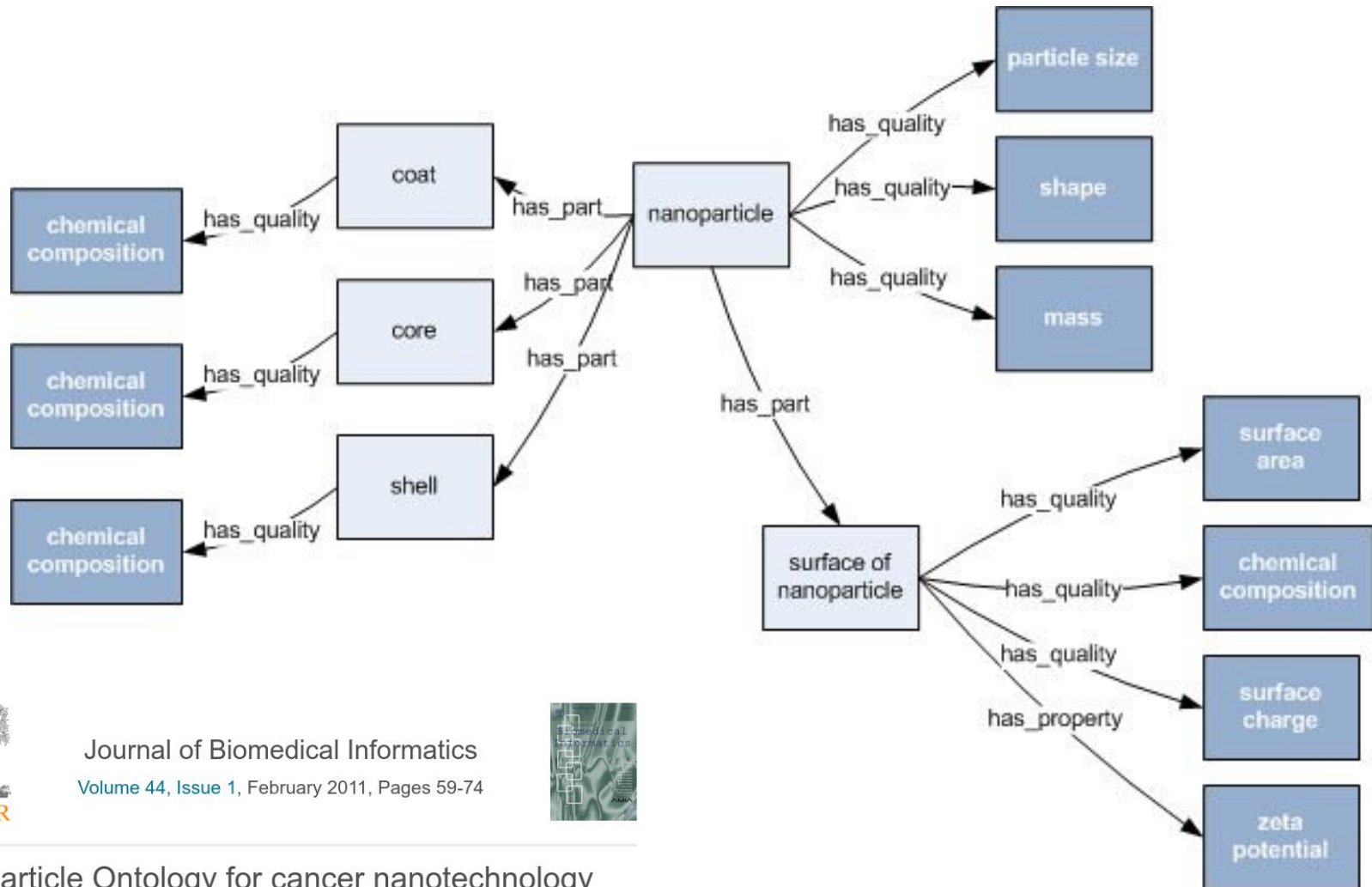
Janna Hastings, Leonid Chepelev, Egon Willighagen, Nico Adams, Christoph Steinbeck, Michel Dumontier

Published: October 3, 2011 • <https://doi.org/10.1371/journal.pone.0025513>

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11,502 View	27 Share



# This NanoParticle Ontology (NPO)



Journal of Biomedical Informatics  
Volume 44, Issue 1, February 2011, Pages 59-74



NanoParticle Ontology for cancer nanotechnology research

Dennis G. Thomas <sup>a, b</sup>, Rohit V. Pappu <sup>b, c</sup>, Nathan A. Baker <sup>a, b</sup> ✉



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# Ontologies and spreadsheets

# What is a spreadsheet?

The screenshot shows a LibreOffice Calc spreadsheet with the following data:

	A	B	C	D	E	F	G	H	I
	label	size (nm)	zeta potential (mV)	cells	exposure time (h)	cell viability	article		
2	CeO2	20.3		L929	24	97.53237	10.1016/j.ceramint.2014.09.095		
3	Se	79.6		0PC3	24	91.09037	10.4172/2157-7439.1000194		



# Supplementary Information

## Meta-Analysis of Nanoparticle Cytotoxicity via Data-Mining the Literature

Hagar I. Labouta\*, Nasimeh Asgarian, Kristina Rinker and David T. Cramb\*

✓ **Cite this:** *ACS Nano* 2019, 13, 2, 1583-1594

Publication Date: January 28, 2019 ✓

<https://doi.org/10.1021/acsnano.8b07562>

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Supporting Info

**SUBJECTS:** [Coating materials](#), [Assays](#), [Toxicity Nanoparticles](#)

### Abstract

Developing predictive modeling frameworks of potential cytotoxicity of engineered nanoparticles is critical for environmental and health risk analysis. The complexity and the heterogeneity of available data on potential risks of nanoparticles, in addition to interdependency of relevant influential attributes, makes it challenging to develop a generalization of nanoparticle toxicity behavior. Lack of

# Problem: Excel dates

Correspondence | [Open Access](#) | Published: 23 June 2004

## Mistaken Identifiers: Gene name errors can be introduced inadvertently when using Excel in bioinformatics

[Barry R Zeeberg](#), [Joseph Riss](#), [David W Kane](#), [Kimberly J Bussey](#), [Edward Uchio](#), [W Marston Linehan](#), [J Carl Barrett](#) & [John N Weinstein](#) 

*BMC Bioinformatics* 5, Article number: 80 (2004) | [Cite this article](#)

114k Accesses | 44 Citations | 514 Altmetric | [Metrics](#)

### Abstract

#### Background

When processing microarray data sets, we recently noticed that some gene names were being changed inadvertently to non-gene names.

#### Results

A little detective work traced the problem to default date format conversions and floating-point format conversions in the very useful Excel program package. The date conversions affect at least 30 gene names; the floating-point conversions affect at least 2,000 if Riken identifiers are included. These conversions are irreversible: the original gene names cannot be

# Mapping the spreadsheet content into the data model


	A	B	C	D	E	F	G
1	<b>TEST RESULTS</b>						
2							
3							
4		Replicate 1				Replicate 2	
5		T1	Titanium Dioxide	Average (ng/ml)		T1	Titanium Dioxide
6			0	1.8925			
7			1	19.6985			
8			5	18.5307			
9			10	18.0280			
10			25	18.4153			
11			50	19.2965			
12			75	20.8867			
13			100	22.6964			
14							
15							
16							



through JSON configuration



```
{
  "TEMPLATE": {
    "DATA": {
      "PARAMETERS": {
        "SUBSTANCE_RECORD": { ... }, // 7 items
        "PROTOCOL_APPLICATIONS": [
          {
            "PROTOCOL_TOP_CATEGORY": { ... }, // 2 items
            "PROTOCOL_CATEGORY_CODE": { ... }, // 2 items
            "PROTOCOL_GUIDELINE": { ... }, // 1 item
            "PROTOCOL_ENDPOINT": { ... }, // 4 items
            "RELIABILITY_STUDY_RESULT_TYPE": { ... }, // 2 items
            "CITATION_TITLE": { ... }, // 2 items
            "CITATION_YEAR": { ... }, // 2 items
            "CITATION_OWNER": { ... }, // 4 items
            "PARAMETERS": { ... }, // 12 items
            "EFFECTS_BLOCK": {
              "LOCATION": {
                "ITERATION": "ABSOLUTE_LOCATION",
                "IS_ARRAY": true,
                "TRIM_ARRAY": true,
                "SHEET_INDEX": 3,
                "COLUMN_INDEX": "B",
                "ROW_INDEX": 4
              },
              "ROW_SUBBLOCKS": "= TimePoints.size()",
              "COLUMN_SUBBLOCKS": "= Replicates",
              "SUBBLOCK_SIZE_ROWS": "= C.size() + 3",
              "SUBBLOCK_SIZE_COLUMNS": 4,
              "VALUE_GROUPS": [
                {
                  "NAME": "=Assay_endpoint",
                  "UNIT": "=Outcome_metric",
                  "START_COLUMN": 3,
                  "END_COLUMN": 3,
                  "START_ROW": 3,
                  "END_ROW": "=3 - 1 + C.size()",
                  "PARAMETERS": [
                    {
                      "NAME": "Time point",
                      "ASSIGN": "ASSIGN_TO_SUBBLOCK",
                      "COLUMN_POS": 1,
                      "ROW_POS": 2,
                      "MAPPING": "Time",
                      "UNIT": "h"
                    },
                    {
                      "NAME": "Replicate",
                      "ASSIGN": "ASSIGN_TO_SUBBLOCK",
                      "COLUMN_POS": 1,
                      "ROW_POS": 1
                    },
                    {
                      "NAME": "Concentration",
                      "ASSIGN": "ASSIGN_TO_VALUE",
                      "COLUMN_POS": -1,
                      "ROW_POS": 0,
                      "UNIT": "Âµg/ml"
                    }
                  ]
                }
              ]
            }
          }
        ]
      }
    }
  }
}
```


← → C <https://apps.ideaconsult.net/enanomapper/ui/uploadsubstance1>

 Search ▾ Nanomaterials ▾ OpenTox ▾ Help ▾

⌂ > Substances > Import > Single file upload

Import new substance(s)

File (.i5z  or .i5d or .xls or .xlsx )\*  No file chosen

JSON map for XLS/XLSX file   No file chosen

# Mapping the spreadsheet content into the data model

```
"CLO_0000031 EF0_0004443" : {  
  "ITERATION": "ABSOLUTE_LOCATION",  
  "SHEET_INDEX": 1,  
  "COLUMN_INDEX": "B",  
  "ROW_INDEX": 49,  
  "original" : "Cell line/Type - Supplier"  
},  
"OBI_0001911 BAO_0000114" : {  
  "ITERATION": "ABSOLUTE_LOCATION",  
  "SHEET_INDEX": 1,  
  "COLUMN_INDEX": "B",  
  "ROW_INDEX": 53,  
  "original" : "Cell culture conditions - Medium"  
},
```

**JSON** (JavaScript Object Notation) is a lightweight data-interchange format.







*nanomaterials*

Supplementary Materials



# Your Spreadsheets Can Be FAIR: A Tool and FAIRification Workflow for the eNanoMapper Database

Nikolay Kochev <sup>1,2,\*</sup>, Nina Jeliazkova <sup>2,\*</sup>, Vesselina Paskaleva <sup>1</sup>, Gergana Tancheva <sup>1</sup>, Luchesar Iliev <sup>2</sup>, Peter Ritchie <sup>3</sup> and Vedrin Jeliazkov <sup>2</sup>

<sup>1</sup> University of Plovdiv, Faculty of Chemistry, Department of Analytical Chemistry and Computer Chemistry, 24 Tsar Assen St. 4000 Plovdiv, Bulgaria; [vesse@uni-plovdiv.net](mailto:vesse@uni-plovdiv.net) (V.P.);

NanoReg<sup>2</sup>



Maastricht University



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# Other ontology use cases

# Search interface and functionalities

Data.enanomapper.net

The image displays the eNanoMapper search interface. On the left, a smaller window shows the 'Welcome to eNanoMapper prototype' page with a search bar and a button labeled 'Try the new free text search application'. A blue arrow points from this button to the main search results page on the right. The main page shows the search results for 'zinc%20oxide'. The left sidebar contains filters for 'Current Selection' (zinc oxide), 'Data sources' (FP7 MARINA, MODENA, NanoWiki), 'Nanomaterial type' (zinc oxide), 'P-CHEM (19)', 'TOX (4)', 'Results', 'References', 'Protocols', 'Instruments', and 'Species'. The main content area displays a list of search results, including 'ZnO NM-110', 'ZnO NM-111', 'JRC2011 NM-111 NM-111', 'Gerloff2009 NM9 ZnO-F', 'Kim2012 NM2 ZnO', 'Gerloff2009 NM7 ZnO', 'Shi2012 NM3 ZnO', 'Lin2011 M4 ZnO', 'Gerloff2009 NM8 ZnO-Ns', and 'Cytotox2011Puzyn01 ZnO'. Each result includes a brief description and a 'more' link.

<https://search.data.enanomapper.net/>

Slide: Dr. Nina Jeliaskova, IdeaConsult Ltd.

# Google Dataset Search: keyword annotation

The screenshot shows the Google Dataset Search interface. At the top, the Google logo is on the left, and a search bar contains the text 'nanowiki'. To the right of the search bar are icons for information, a chat bubble, a grid, and a user profile. Below the search bar, there are four filter buttons: 'Updated date', 'Download format', 'Usage rights', and 'Free'. The search results are displayed in two columns. The left column, titled '5 data sets found', lists four datasets: 'Data from: NanoWiki (release 1)' (figshare.com, updated Jan 19, 2016), 'NanoWiki 5' (figshare.com, updated Sep 11, 2018), 'NanoWiki (release 4)' (figshare.com, updated Nov 6, 2016), and 'NanoWiki (release 3)' (figshare.com, updated May 14, 2016). The right column provides detailed information for the first dataset, 'Data from: NanoWiki (release 1)'. It includes a 'Related Article' link, a blue button to 'Explore at figshare.com', a 'Unique identifier' with a DOI link, a 'Data set updated' date, 'Data set provided by' (figshare), 'Authors' (Egon Willighagen), 'Licence' (Attribution 4.0 (CC BY 4.0)), and 'Available download formats from providers' (application/gzip).

Google

nanowiki

Updated date Download format Usage rights Free

5 data sets found

**Data from: NanoWiki (release 1)**  
figshare.com  
Updated Jan 19, 2016

**NanoWiki 5**  
figshare.com  
search.datacite.org  
Updated Sep 11, 2018

**NanoWiki (release 4)**  
figshare.com  
search.datacite.org  
Updated Nov 6, 2016

**NanoWiki (release 3)**  
figshare.com  
Updated May 14, 2016

**Data from: NanoWiki (release 1)**

Related Article

Explore at figshare.com

**Unique identifier**  
<https://doi.org/10.6084/m9.figshare.1330208.v1>

**Data set updated** Jan 19, 2016

**Data set provided by**  
figshare

**Authors**  
Egon Willighagen

**Licence**  
[Attribution 4.0 \(CC BY 4.0\)](#)  
Licence information was derived automatically

**Available download formats from providers**  
application/gzip










# Bioschemas Dataset Profile

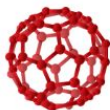
## Compliant with Google Dataset Profile

- 5 minimal properties
- 8 recommended properties
  - Link to DataCatalog
  - Link to DataDownload

<https://bioschemas.org/profiles/Dataset/>

 <a href="#">Home</a> <a href="#">Join</a> <a href="#">Meetings</a> <a href="#">Specifications</a> <a href="#">Software</a> <a href="#">About</a>					
Property	Expected Type	Description	CD	Controlled Vocabulary	Example
Marginality: Minimum.					
<a href="#">description</a>	<a href="#">Text</a>	<b>Schema:</b> A description of the item.  <b>Bioschemas:</b> A short summary describing a dataset.	ONE		
<a href="#">identifier</a>	<a href="#">Property/Value</a> <a href="#">Text</a> <a href="#">URL</a>	<b>Schema:</b> The identifier property represents any kind of identifier for any kind of Thing, such as ISBNs, GTIN codes, UUIDs etc. Schema.org provides dedicated properties for representing many of these, either as textual strings or as URL (URI) links. See <a href="#">background notes</a> for more details.	MANY		
<a href="#">keywords</a>	<a href="#">Text</a>	<b>Schema:</b> Keywords or tags used to describe this content. Multiple entries in a keywords list are typically delimited by commas.  <b>Bioschemas:</b> These keywords provide a summary of the dataset.	MANY		
<a href="#">name</a>	<a href="#">Text</a>	<b>Schema:</b> The name of the item.  <b>Bioschemas:</b> A descriptive name of the dataset.	ONE		
<a href="#">url</a>	<a href="#">URL</a>	<b>Schema:</b> URL of the item.  <b>Bioschemas:</b> The location of a page describing the dataset.	ONE		
Marginality: Recommended.					
<a href="#">citation</a>	<a href="#">CreativeWork</a> <a href="#">Text</a>	<b>Schema:</b> A citation or reference to another creative work, such as another publication, web page, scholarly article, etc.  <b>Bioschemas:</b> A citation for a publication that describes the dataset.	MANY		

# F1: persistent identifiers



## eNanoMapper Ontology IRIs for the OECD nanomaterials

eNanoMapper Working Draft 18 October 2017

**This version:**

<http://specs.enanomapper.org/2017/WD-oecd-20171018/>

**Latest published version:**

<http://specs.enanomapper.org/oecd/>

**Previous version:**

none

**Editor:**

[Egon Willighagen](#), [Maastricht University](#)

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### Abstract

OECD nanomaterial	Code	Full Ontology IRI
cerium oxide nanoparticles	ENM_9000006	<a href="http://purl.enanomapper.org/onto/ENM_9000006">http://purl.enanomapper.org/onto/ENM_9000006</a>
multi-walled carbon nanotubes	NPO_354	<a href="http://purl.bioontology.org/ontology/npo#NPO_354">http://purl.bioontology.org/ontology/npo#NPO_354</a>
single-walled carbon nanotubes	NPO_943	<a href="http://purl.bioontology.org/ontology/npo#NPO_943">http://purl.bioontology.org/ontology/npo#NPO_943</a>
dendrimers	NPO_735	<a href="http://purl.bioontology.org/ontology/npo#NPO_735">http://purl.bioontology.org/ontology/npo#NPO_735</a>
nanoclay nanoparticles	ENM_9000007	<a href="http://purl.enanomapper.org/onto/ENM_9000007">http://purl.enanomapper.org/onto/ENM_9000007</a>
titanium dioxide nanoparticles	CHEBI_51050	<a href="http://purl.obolibrary.org/obo/CHEBI_51050">http://purl.obolibrary.org/obo/CHEBI_51050</a>
fullerenes	CHEBI_33128	<a href="http://purl.obolibrary.org/obo/CHEBI_33128">http://purl.obolibrary.org/obo/CHEBI_33128</a>
silicon dioxide nanoparticles	NPO_1373	<a href="http://purl.bioontology.org/ontology/npo#NPO_1373">http://purl.bioontology.org/ontology/npo#NPO_1373</a>
zinc oxide nanoparticles	NPO_1542	<a href="http://purl.bioontology.org/ontology/npo#NPO_1542">http://purl.bioontology.org/ontology/npo#NPO_1542</a>
gold nanoparticles	NPO_401	<a href="http://purl.bioontology.org/ontology/npo#NPO_401">http://purl.bioontology.org/ontology/npo#NPO_401</a>
silver nanoparticles	NPO_1892	<a href="http://purl.bioontology.org/ontology/npo#NPO_1892">http://purl.bioontology.org/ontology/npo#NPO_1892</a>
iron nanoparticles	ENM_9000200	<a href="http://purl.enanomapper.org/onto/ENM_9000200">http://purl.enanomapper.org/onto/ENM_9000200</a>
aluminium oxide nanoparticles	ENM_9000005	<a href="http://purl.enanomapper.org/onto/ENM_9000005">http://purl.enanomapper.org/onto/ENM_9000005</a>





# Ontology IRIs for the JRC representative industrial

NanoCommons Working Draft 26 June 2020

## This version:

<http://nanocommons.github.io/specifications/2020/WD-jrc-20200626/>

## Latest published version:

<http://nanocommons.github.io/specifications/jrc/>

## Previous version:

<http://nanocommons.github.io/specifications/2020/WD-jrc-20200517/>

## Editor:

[Egon Willighagen](#), [Maastricht University](#)

## Author:

Jiakang Chang, [EMBL-EBI](#)

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## Abstract

The [JRC representative industrial nanomaterials](#) are a series of nanomaterials used [NanoCommons](#) is developing an ontology to be used as common language by this ontology and provides identifiers for each of them. It is based on an earlier specification <https://enanomapper.github.io/specifications/jrc/>. The sources can be found at <https://enanomapper.github.io/specifications/jrc/>.

## 2. The mappings

The below table gives the ontology IRIs for each of the JRC representative nanomaterials. Import synonyms; these are explicitly different in the ontology.

JRC nanomaterial Code	Ontology IRI	Wikidata
JRCNM01000a	ENM_9000074 <a href="http://purl.enanomapper.org/onto/ENM_9000074">http://purl.enanomapper.org/onto/ENM_9000074</a>	<a href="#">Q27918612</a>
JRCNM01001a	ENM_9000075 <a href="http://purl.enanomapper.org/onto/ENM_9000075">http://purl.enanomapper.org/onto/ENM_9000075</a>	<a href="#">Q47461406</a>
JRCNM01002a	ENM_9000076 <a href="http://purl.enanomapper.org/onto/ENM_9000076">http://purl.enanomapper.org/onto/ENM_9000076</a>	<a href="#">Q47461416</a>
JRCNM01003a	ENM_9000083 <a href="http://purl.enanomapper.org/onto/ENM_9000083">http://purl.enanomapper.org/onto/ENM_9000083</a>	<a href="#">Q47461418</a>
JRCNM01004a	ENM_9000084 <a href="http://purl.enanomapper.org/onto/ENM_9000084">http://purl.enanomapper.org/onto/ENM_9000084</a>	<a href="#">Q47461419</a>
JRCNM01005a	ENM_9000077 <a href="http://purl.enanomapper.org/onto/ENM_9000077">http://purl.enanomapper.org/onto/ENM_9000077</a>	<a href="#">Q47461422</a>
JRCNM01100a	ENM_9000078 <a href="http://purl.enanomapper.org/onto/ENM_9000078">http://purl.enanomapper.org/onto/ENM_9000078</a>	<a href="#">Q47462004</a>
JRCNM01101a	ENM_9000086 <a href="http://purl.enanomapper.org/onto/ENM_9000086">http://purl.enanomapper.org/onto/ENM_9000086</a>	<a href="#">Q47462008</a>
JRCNM02000a	ENM_9000087 <a href="http://purl.enanomapper.org/onto/ENM_9000087">http://purl.enanomapper.org/onto/ENM_9000087</a>	<a href="#">Q47462022</a>
JRCNM02001a	ENM_9000088 <a href="http://purl.enanomapper.org/onto/ENM_9000088">http://purl.enanomapper.org/onto/ENM_9000088</a>	<a href="#">Q47468470</a>
JRCNM02002a	ENM_9000089 <a href="http://purl.enanomapper.org/onto/ENM_9000089">http://purl.enanomapper.org/onto/ENM_9000089</a>	<a href="#">Q47468473</a>
JRCNM02003a	ENM_9000090 <a href="http://purl.enanomapper.org/onto/ENM_9000090">http://purl.enanomapper.org/onto/ENM_9000090</a>	<a href="#">Q78642247</a>
JRCNM02004a	ENM_9000091 <a href="http://purl.enanomapper.org/onto/ENM_9000091">http://purl.enanomapper.org/onto/ENM_9000091</a>	<a href="#">Q47468478</a>
JRCNM02004b	ENM_9000092 <a href="http://purl.enanomapper.org/onto/ENM_9000092">http://purl.enanomapper.org/onto/ENM_9000092</a>	<a href="#">Q78642927</a>
JRCNM02101a	ENM_9000237 <a href="http://purl.enanomapper.org/onto/ENM_9000237">http://purl.enanomapper.org/onto/ENM_9000237</a>	<a href="#">Q78643426</a>
JRCNM02102a	ENM_9000238 <a href="http://purl.enanomapper.org/onto/ENM_9000238">http://purl.enanomapper.org/onto/ENM_9000238</a>	<a href="#">Q47461933</a>
JRCNM03000a	ENM_9000255 <a href="http://purl.enanomapper.org/onto/ENM_9000255">http://purl.enanomapper.org/onto/ENM_9000255</a>	<a href="#">Q94632421</a>
JRCNM03300a	ENM_9000097 <a href="http://purl.enanomapper.org/onto/ENM_9000097">http://purl.enanomapper.org/onto/ENM_9000097</a>	<a href="#">Q58631733</a>
JRCNM03301a	ENM_9000098 <a href="http://purl.enanomapper.org/onto/ENM_9000098">http://purl.enanomapper.org/onto/ENM_9000098</a>	<a href="#">Q78598603</a>
JRCNM04000a	ENM_9000080 <a href="http://purl.enanomapper.org/onto/ENM_9000080">http://purl.enanomapper.org/onto/ENM_9000080</a>	<a href="#">Q47462019</a>
JRCNM04001a	ENM_9000081 <a href="http://purl.enanomapper.org/onto/ENM_9000081">http://purl.enanomapper.org/onto/ENM_9000081</a>	<a href="#">Q47462603</a>
JRCNM50001a	ENM_9000256 <a href="http://purl.enanomapper.org/onto/ENM_9000256">http://purl.enanomapper.org/onto/ENM_9000256</a>	<a href="#">Q94632692</a>
JRCNM10200a	ENM_9000231 <a href="http://purl.enanomapper.org/onto/ENM_9000231">http://purl.enanomapper.org/onto/ENM_9000231</a>	<a href="#">Q87125303</a>
JRCNM10201a	ENM_9000094 <a href="http://purl.enanomapper.org/onto/ENM_9000094">http://purl.enanomapper.org/onto/ENM_9000094</a>	<a href="#">Q78603081</a>
JRCNM10202a	ENM_9000232 <a href="http://purl.enanomapper.org/onto/ENM_9000232">http://purl.enanomapper.org/onto/ENM_9000232</a>	<a href="#">Q87124091</a>
JRCNM10404	ENM_9000093 <a href="http://purl.enanomapper.org/onto/ENM_9000093">http://purl.enanomapper.org/onto/ENM_9000093</a>	<a href="#">Q58630711</a>
JRCNM62001a	ENM_9000095 <a href="http://purl.enanomapper.org/onto/ENM_9000095">http://purl.enanomapper.org/onto/ENM_9000095</a>	<a href="#">Q75188647</a>
JRCNM62002a	ENM_9000096 <a href="http://purl.enanomapper.org/onto/ENM_9000096">http://purl.enanomapper.org/onto/ENM_9000096</a>	<a href="#">Q75188523</a>
JRCNM62101a	ENM_9000079 <a href="http://purl.enanomapper.org/onto/ENM_9000079">http://purl.enanomapper.org/onto/ENM_9000079</a>	<a href="#">Q75188316</a>

# Bioschemas JSON-LD markup

```
<table>
  <tr>
    <td style="font-weight: bold">JRC nanomaterial</td>
    <td style="font-weight: bold">Code</td>
    <td style="font-weight: bold">Ontology IRI</td>
    <td style="font-weight: bold">Wikidata</td>
    <td style="font-weight: bold">Compact Identifier</td>
  </tr>
  <tr>
    <td>JRCNM01000a<script type="application/ld+json">{"@context": "https://schema.org/", "@type":
"ChemicalSubstance", "name": "JRCNM01000a", "identifier": "ENM_9000074", "url": [
"https://scholia.toolforge.org/Q27918612", "http://bioportal.bioontology.org/ontologies/ENM/?
p=classes&conceptid=http%3A%2F%2Fpurl.enanmapper.org%2Fonto%2FENM_9000074"] }</script></td>
    <td>ENM_9000074</td>
    <td><a href="http://bioportal.bioontology.org/ontologies/ENM/?
p=classes&conceptid=http%3A%2F%2Fpurl.enanmapper.org%2Fonto%2FENM_9000074">http://purl.enanmapper.org/onto/
74</a></td>
    <td><a href="https://scholia.toolforge.org/Q27918612">Q27918612</a></td>
    <td>wikidata:Q27918612</td>
  </tr>
  <tr>
    <td>JRCNM01001a<script type="application/ld+json">{"@context": "https://schema.org/", "@type":
"ChemicalSubstance", "name": "JRCNM01001a", "identifier": "ENM_9000075", "url": [
"https://scholia.toolforge.org/Q47461406", "http://bioportal.bioontology.org/ontologies/ENM/?
p=classes&conceptid=http%3A%2F%2Fpurl.enanmapper.org%2Fonto%2FENM_9000075"] }</script></td>
    <td>ENM_9000075</td>
```

# Bioschemas JSON-LD markup

```
{
  "@context": "https://schema.org/",
  "@type": "ChemicalSubstance",
  "name": "JRCNM01000a",
  "identifier": "ENM_9000074",
  "url": [
    "https://scholia.toolforge.org/Q27918612",
    "http://bioportal.bioontology.org/ontologies/ENM/?p=classes&conceptid=http%3A%2F%2Fpurl.enanomapper.org%2Fonto%2FENM_9000074"
  ]
}
```

# Acknowledgments

- [eNanoMapper](#), EC FP7, #604134
  - Janna Hastings
- [NanoCommons](#), EC H2020, #731032
- [OpenRiskNet](#), EC H2020, #731075  
(and all partners)
- [EU NanoSafety Cluster](#) (particularly WG F, formerly WG 4)
- [US Nano WG](#)



eNanoMapper Ontology IRIs for the JRC representative industrial nanomaterials

eNanoMapper Working Draft 20 January 2018

**This version:**  
<http://specs.enanomapper.org/2018/WD-rc-20180120/>  
**Latest published version:**  
<http://specs.enanomapper.org/jrc/>  
**Previous version:**  
<http://specs.enanomapper.org/2017/WD-rc-20170226/>  
**Editor:**  
 Egon Willighagen, Maastricht University  
**Author:**  
 Jiakang Chang, EMBL-FBI

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## Abstract

The JRC representative industrial nanomaterials are a series of nanomaterials used in the European nanosafety community for research [Tixaro2016]. 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. The sources can be found at <https://github.com/enanomapper/specifications>.



eNanoMapper Ontology IRIs for the OECD nanomaterials

eNanoMapper Working Draft 18 October 2017

**This version:**  
<http://specs.enanomapper.org/2017/WD-oecd-20171018/>  
**Latest published version:**  
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**Previous version:**  
 none  
**Editor:**  
 Egon Willighagen, Maastricht University

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## 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.

The screenshot shows the EUON website interface. At the top, there's a navigation bar with 'General Information', 'Uses', 'Safety', 'Regulation', 'International activities', and 'Research & Innovation'. Below this, a search bar is visible. The main content area displays search results for 'JRCNM4001a (NM-401 (MWCNT 64.2 nm)) multi-walled carbon nanotube'. It lists various properties and data sources, including 'P-CHEM Crystalline phase', 'P-CHEM Surface chemistry', 'P-CHEM Particle size distribution', 'P-CHEM Batch Dispersion quality', 'P-CHEM Outlines', 'P-CHEM Specific surface area', 'TOX Immunotoxicity', 'TOX Cell Viability', 'TOX Genetic toxicity in vitro', 'ECOTOX Short-term toxicity to aquatic invertebrates', 'TOX Repeated dose toxicity - oral', 'P-CHEM Zeta potential', and 'P-CHEM Aerosol characterisation'. There are also links for 'Substance', 'Composition', and 'Study'. A second result for 'JRCNM4002a (NM-402 (MWCNT 12.7 nm)) multi-walled carbon nanotube' is partially visible below.



# Ontologies define hierarchies (also)

## metal oxide nanoparticle

- aluminium oxide nanoparticle
- cadmium(II) oxide nanoparticle
- cerium oxide nanoparticle
- copper oxide nanoparticle
- copper(II) oxide nanoparticle
- europium trioxide nanoparticle
- iron oxide nanoparticle
  - dextran-coated iron oxide nanoparticle
  - hematite nanoparticle
  - iron (II,III) oxide nanoparticle
  - iron (III) oxide nanoparticle
  - magnetite nanoparticle
  - superparamagnetic iron oxide nanoparticle
- manganese (IV) dioxide nanoparticle
- molybdenum trioxide nanoparticle

- transferase activity assay

## gene expression assay

- reporter gene assay
- transcriptional response profiling assay

## genotoxicity assay

- DNA Damage Assay
- ion channel assay
- localization assay
- membrane potential assay
  - ion channel assay
  - mitochondrial membrane potential assay
  - nuclear membrane potential assay
  - plasma membrane potential assay
- metastasis assay
- organism behavior assay



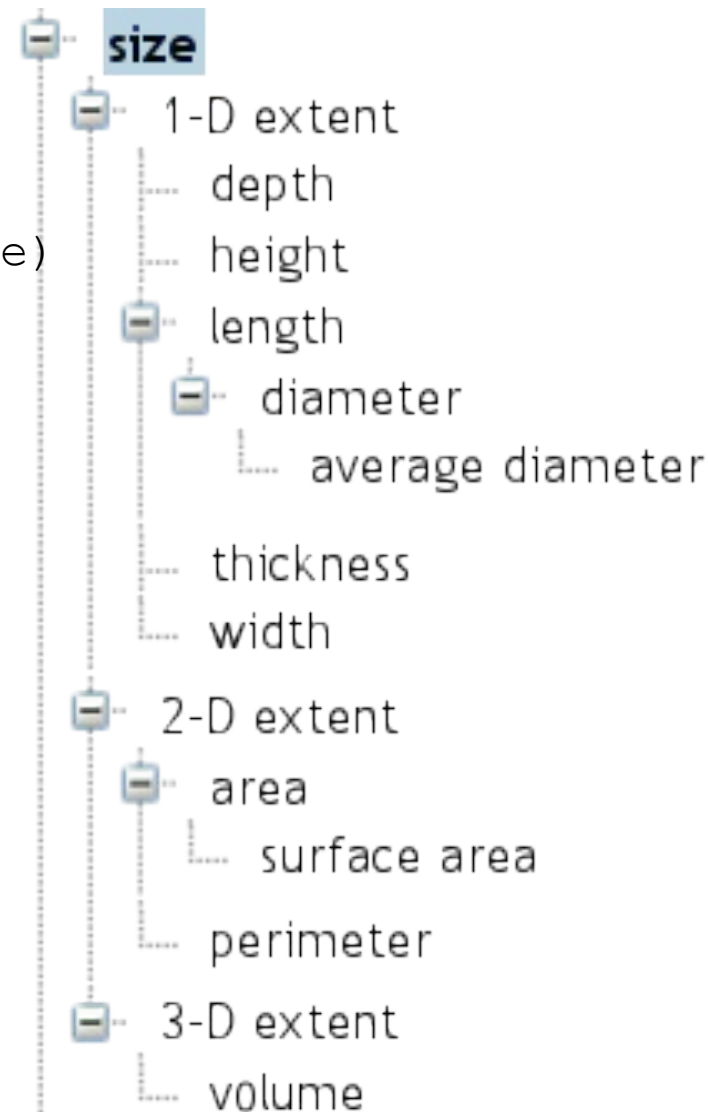
# All metal oxides showing genotoxicity

Which metal oxides (*NPO\_1541*) show a form of genotoxicity (*BAO\_0002167*)?

substance	particleType	experiment	protocol	value	unit
Gerloff2009 NM2	titanium oxide nanoparticle	DNA in Tail	Fpg-2Dmodified Comet Assay	6.0	%
Gerloff2009 NM2	titanium oxide nanoparticle	DNA in Tail	Fpg-2Dmodified Comet Assay	5.0	%
Gerloff2009 NM2	titanium oxide nanoparticle	DNA in Tail	Fpg-2Dmodified Comet Assay	8.0	%
Gerloff2009 NM2	titanium oxide nanoparticle	DNA in Tail	Fpg-2Dmodified Comet Assay	3.0	%
TiO2	titanium oxide nanoparticle	DNA in Tail	Fpg-2Dmodified Comet Assay	6.0	%
TiO2	titanium oxide nanoparticle	DNA in Tail	Fpg-2Dmodified Comet Assay	5.0	%
TiO2	titanium oxide nanoparticle	DNA in Tail	Fpg-2Dmodified Comet Assay	8.0	%
TiO2	titanium oxide nanoparticle	DNA in Tail	Fpg-2Dmodified Comet Assay	3.0	%
ZnO	zinc oxide nanoparticle	DNA in Tail	Fpg-2Dmodified Comet Assay	23.0	%

# Results: data completeness

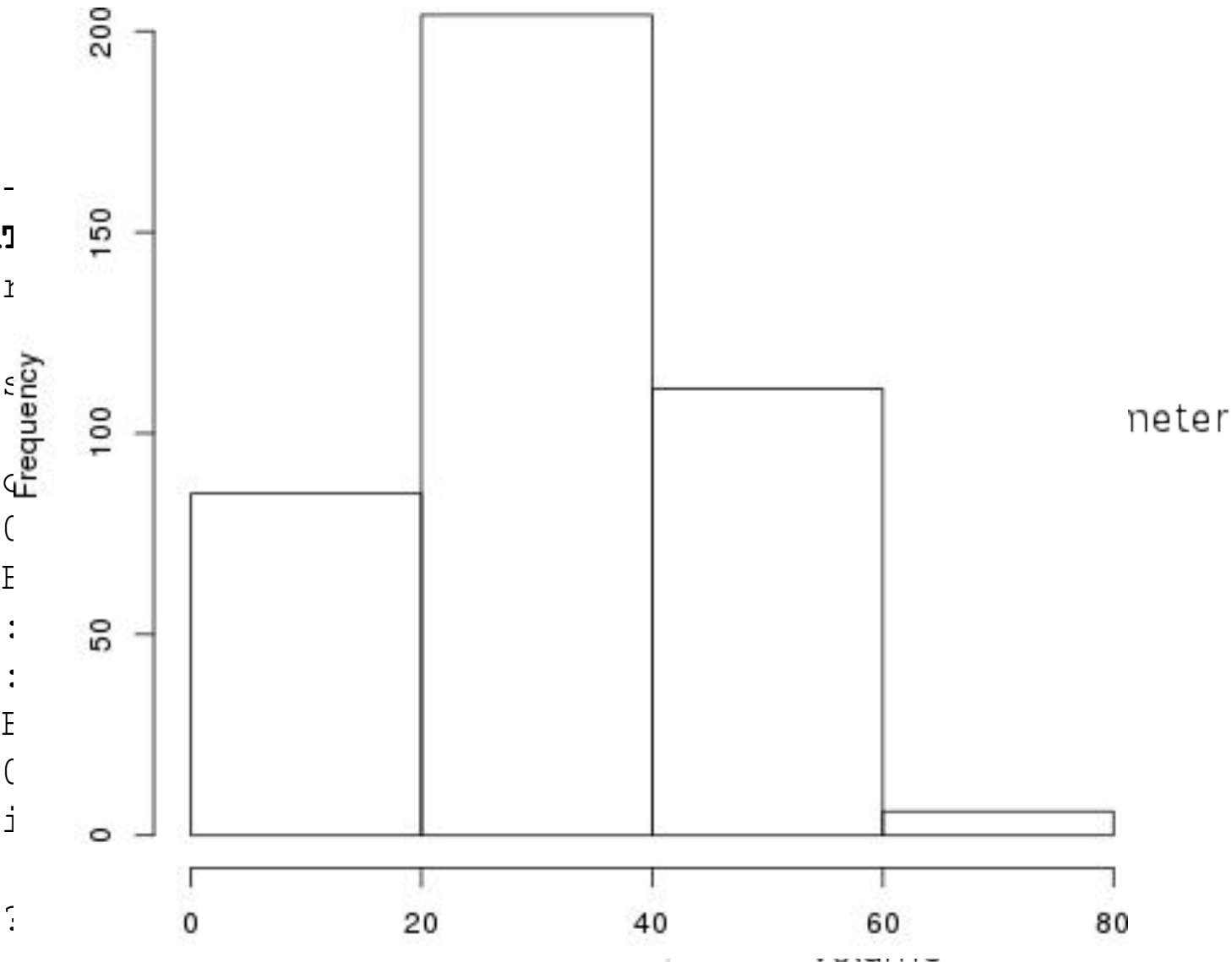
```
SELECT DISTINCT ?substance ?type
              ?title ?value ?unit
WHERE {
  BIND (ex:NWKI-002f5129 AS ?substance)
  BIND (pato:PATO_0000117 as ?propertyType)
  { ?assay a ?propertyType . } UNION
  { ?assay a [
    rdfs:subClassOf+ ?propertyType
  ] }
  ?substance a obo:CHEBI_59999 ;
    obo:BFO_0000056 ?mgroup .
  ?mgroup obo:OBI_0000299 ?endpoint .
  ?endpoint sso:has-value ?value ;
    sso:has-unit ?unit .
  ?assay a bao:BAO_0000015, ?type ;
    bao:BAO_0000209 ?mgroup ;
    dc:title ?title .
  FILTER (?type != bao:BAO_0000015)
} ORDER BY ASC(?substance)
```



# Results: data completeness

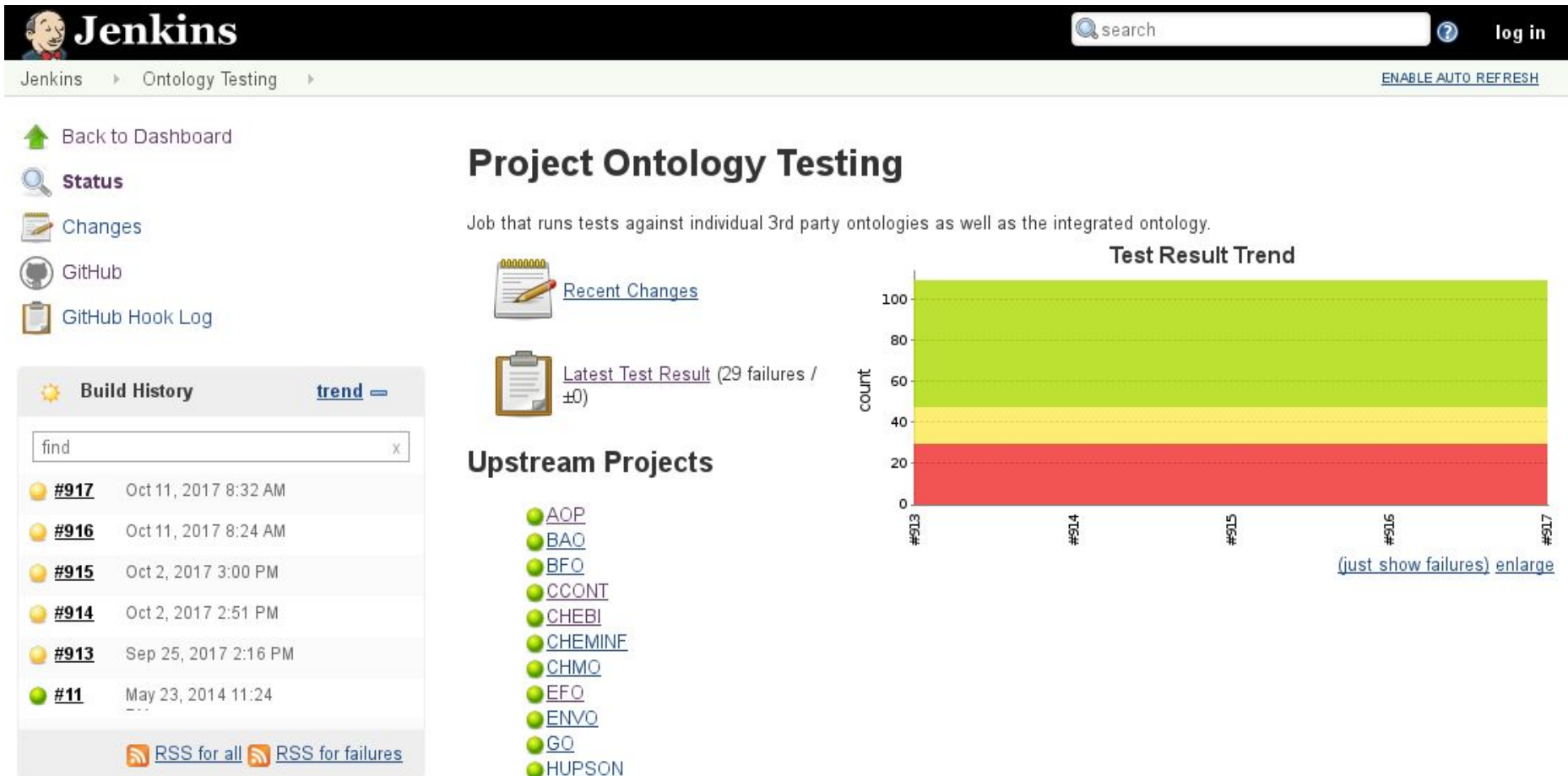
```
SELECT DISTINCT
WHERE {
  BIND (ex:NWKI-
  BIND (pato:PAI
  { ?assay a ?pr
  { ?assay a [
    rdfs:subClas
  ] }
  ?substance a c
    obo:BFO_000(
  ?mgroupp obo:OE
  ?endpoint sso:
    sso:
  ?assay a bao:E
    bao:BAO_000(
    dc:title ?ti
  FILTER (?type
} ORDER BY ASC(?

```



# How we maintain it

# Automatic building: Jenkins





# Building with *Slimmer* and ROBOT

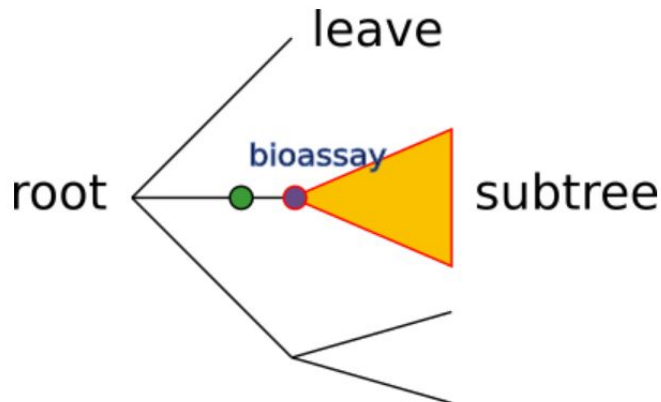
- Configuration to slice upstream ontologies (with OWLAPI)

## The Syntax

Each instruction has the same structure, the same syntax, organized in layers:

D([http://purl.obolibrary.org/obo/OBI\\_0000070](http://purl.obolibrary.org/obo/OBI_0000070)):[http://www.bioassayontology.org/bao#BAO\\_0000015](http://www.bioassayontology.org/bao#BAO_0000015) bioassay

We can see here basically the five layers (red, yellow, green, purple, and blue) and in semi-colon (light blue) to separate two layers. If you consider that an ontology is often a hierarchical tree of terms, with one root node, spreading down, ending in leave nodes, the above instruction could be visualized as this:



Hastings, J.; Jeliaskova, N.; Owen, G.; Tsiliki, G.; Munteanu, C. R.; Steinbeck, C.; Willighagen, E. eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment. J. Biomed. Semantics 2015, 6, 10 DOI: [10.1186/s13326-015-0005-5](https://doi.org/10.1186/s13326-015-0005-5).

# Ontologies to support FAIR research output

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*Nanosafety and the semantic web: from natural language  
to computational processing*

Zoom, 2021-12-8/9