

# *The eNanoMapper Ontology*

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Nanotechnology Working Group (NanoWG) webinar  
8th of December 2016, 17:00-18:00 CET



# What is an ontology and why do we use it?

## Definition:

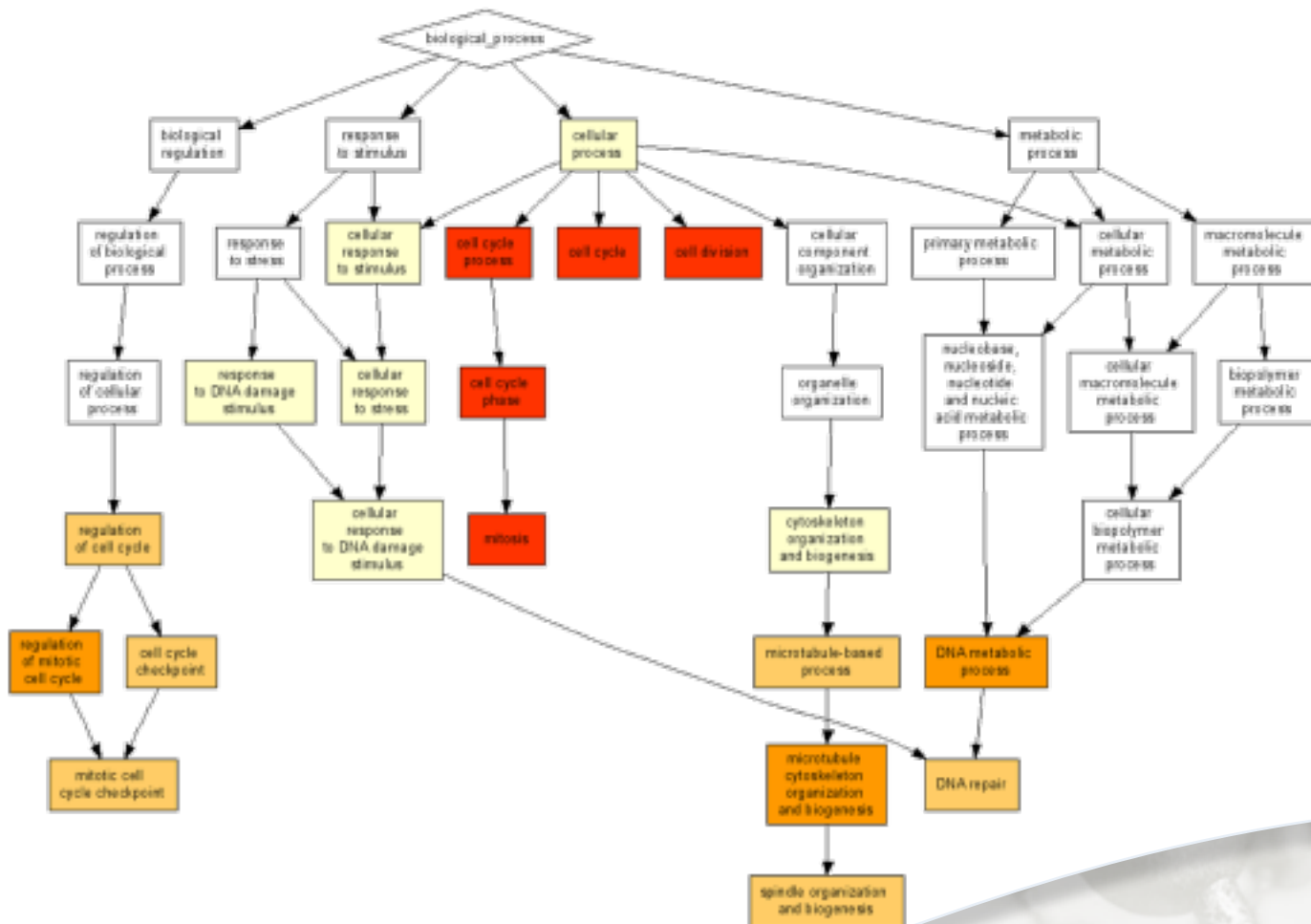
- Standardized, relational controlled vocabulary.
- Complex knowledge representation with relationships, rules and restrictions.

## Usage:

- Harmonize data
- Federated SPARQL queries



# THE example : GENEONTOLOGY



# Development of eNanoMapper (ENM) ontology

- Why reuse?

- Annotations in existing ontologies reused
- Integration of fragmented annotations ≠ possible
- Do not reinvent the wheel
- Feedback to original external ontologies



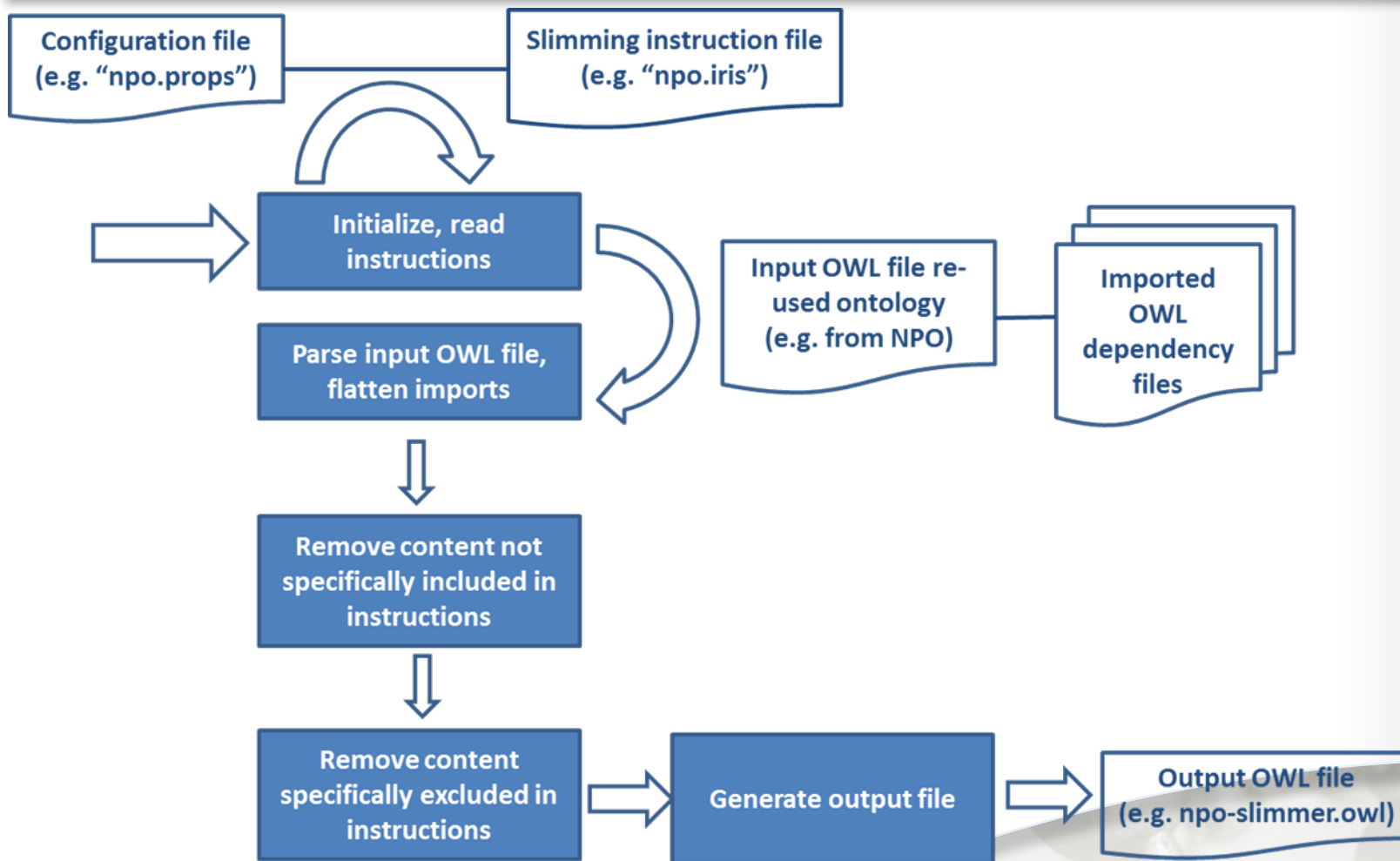
# Reused external ontologies

**Version 3 of the eNM ontology contains 21 external ontology sources**

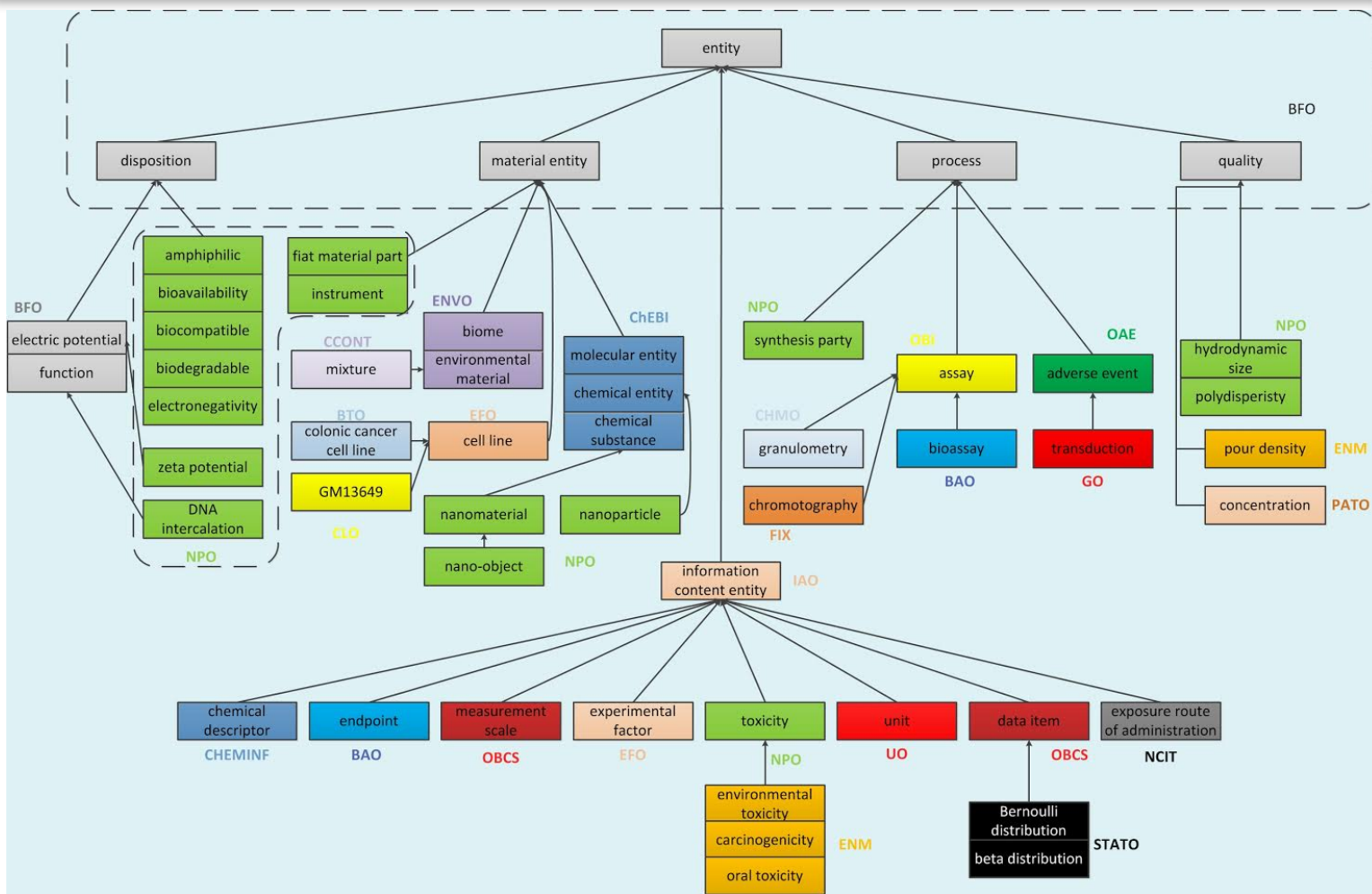
BAO	Bioassay Ontology	GO	Gene Ontology
BFO	Basic Formal Ontology	IAO	Information Artifact Ontology
BTO	BRENDA Tissue and Enzyme Source Ontology	NCIT	National Cancer Institute Thesaurus
CCONT	Cell Culture Ontology	NPO	NanoParticle Ontology
CHEBI	Chemical Entities of Biological Interest	OAE	Ontology of Adverse Events
CHEMINF	Chemical Information Ontology	OBCS	Ontology of Biological and Clinical Statistics
CHMO	Chemical Methods Ontology	OBI	Ontology for Biomedical Investigation
CLO	Cell Line Ontology	PATO	Phenotype quality Ontology
EFO	Experimental Factor Ontology	STATO	Statistics Ontology
ENVO	Environment Ontology	UO	Unit of Measurements Ontology
FIX	Physico-Chemical Methods and Properties		



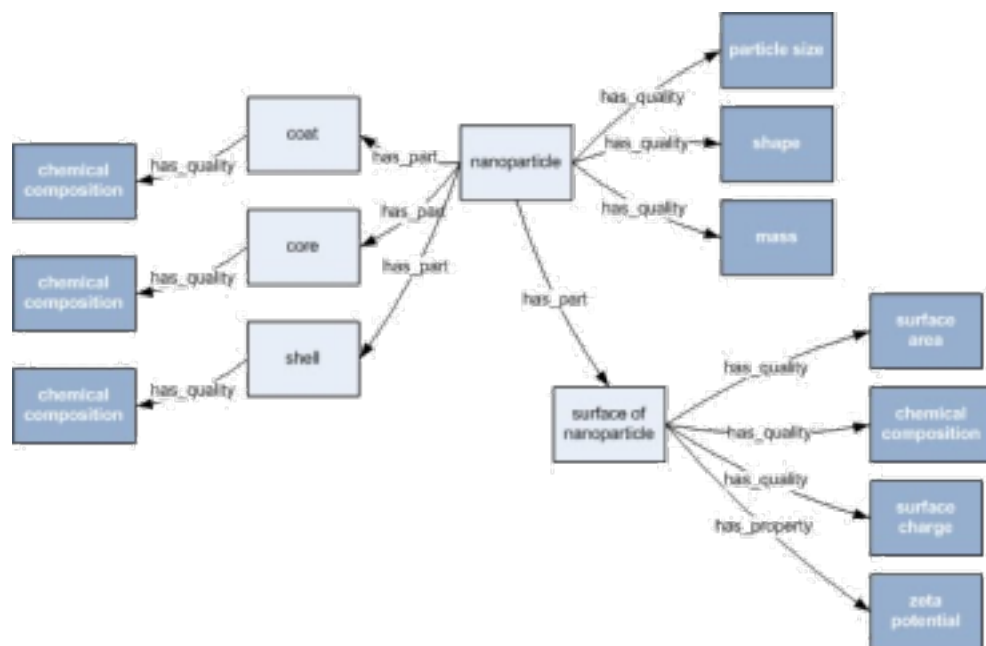
# Slimming procedure – “Only grab what is necessary”



# eNanoMapper Ontology v.3.



# Re-use of NanoParticle Ontology (NPO)





# Browsing the eNanoMapper Ontology

## Online:

### Three main ontology repositories:

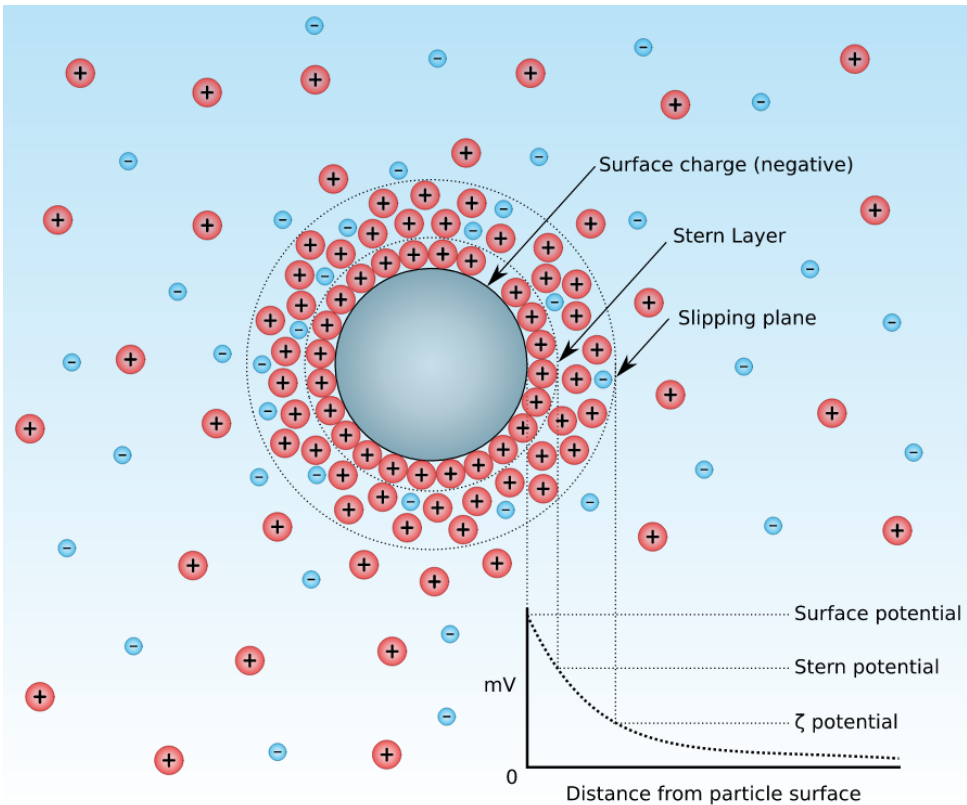
- BioPortal <http://bioportal.bioontology.org/ontologies/ENM>
- Aber-OWL <http://aber-owl.net/ontology/ENM>
- Ontology Lookup Service (OLS)  
<http://www.ebi.ac.uk/ols/beta/ontologies/enm>

## Locally:

- Protégé <http://protege.stanford.edu/>
  - Open from local .owl file
  - Open from URL



# Example: zeta potential



## Definition:

According to Wikipedia:  
*scientific term for electrokinetic potential in colloidal dispersions*



# Online browsing of eNM ontology

# ENM in BioPortal

<http://bioportal.bioontology.org/ontologies/ENM>

BioPortal [Browse](#) [Search](#) [Mappings](#) [Recommender](#) [Annotator](#) [Resource Index](#) [Projects](#) [Recent](#)

## eNanoMapper

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

Jump To:

- entity
  - disposition
    - amphiphilic
    - application
    - bioavailability
    - biocompatible
    - biodegradable
    - electric potential
      - zeta potential**
    - electronegativity
  - function
  - surface property
  - information content entity
  - material entity
  - process
  - quality

Details Visualization Notes ( 0 ) Class Mappings ( 3 ) [↗](#)

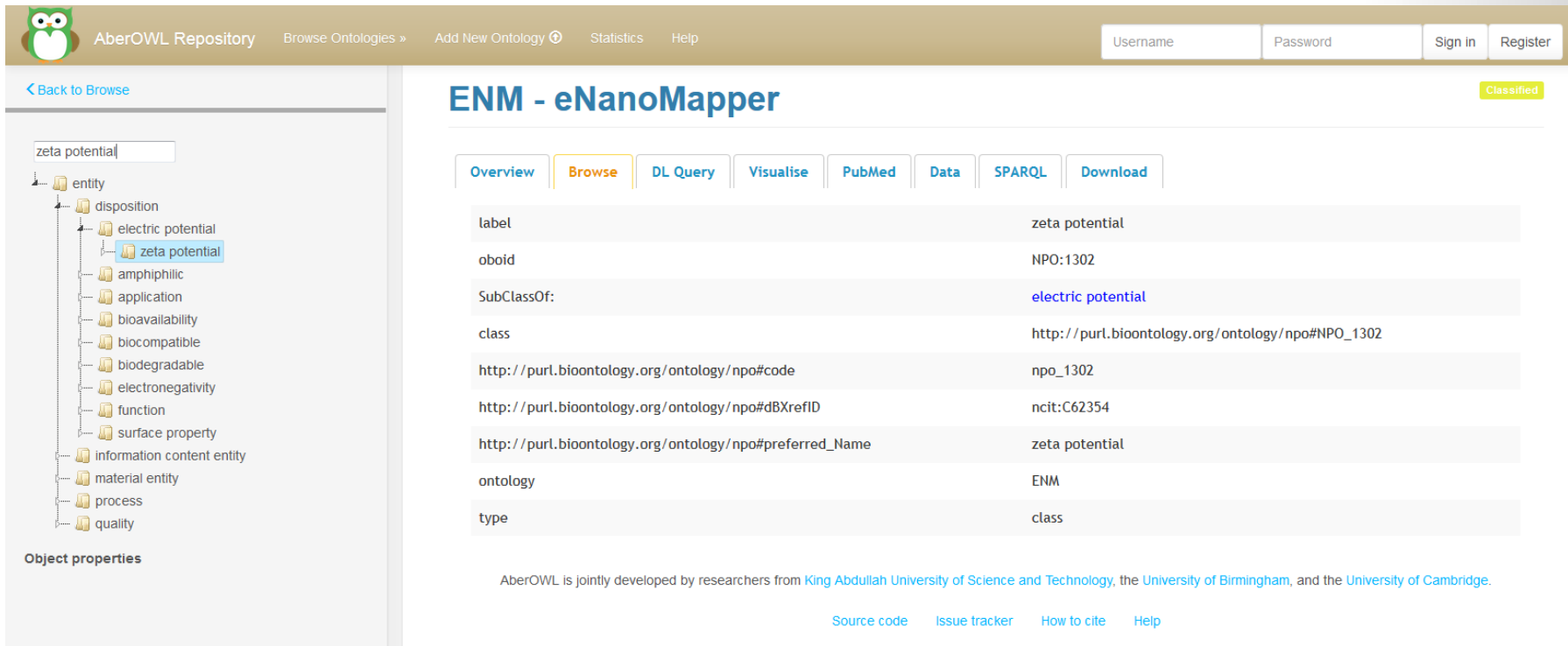
Preferred Name	zeta potential
ID	<a href="http://purl.bioontology.org/ontology/npo#NPO_1302">http://purl.bioontology.org/ontology/npo#NPO_1302</a>
code	NPO_1302
dBxrefID	NCIT:C62354
label	zeta potential
preferred_Name	zeta potential
prefixIRI	<a href="http://purl.bioontology.org/ontology/npo#NPO_1302">npo:NPO_1302</a>
prefLabel	zeta potential
subClassOf	<a href="#">electric potential</a>

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# ENM in Aber-OWL

<http://aber-owl.net/ontology/ENM>



The screenshot shows the AberOWL Repository interface. The top navigation bar includes 'AberOWL Repository', 'Browse Ontologies', 'Add New Ontology', 'Statistics', and 'Help'. There are input fields for 'Username' and 'Password', and buttons for 'Sign in' and 'Register'. The main content area is titled 'ENM - eNanoMapper' and includes a 'Classified' badge. Below the title are tabs for 'Overview', 'Browse', 'DL Query', 'Visualise', 'PubMed', 'Data', 'SPARQL', and 'Download'. A table displays ontology details for 'zeta potential', including its label, oboid (NPO:1302), subclass (electric potential), class URI, and other identifiers. A sidebar on the left shows a tree view of the ontology hierarchy, with 'zeta potential' selected under the 'entity' category. At the bottom, there is a footer with the date '8 December 2016', the European Union flag, and the ENM eNanoMapper logo.

zeta potential

entity

- disposition
  - electric potential
    - zeta potential**
  - amphiphilic
  - application
  - bioavailability
  - biocompatible
  - biodegradable
  - electronegativity
  - function
  - surface property
- information content entity
- material entity
- process
- quality

Object properties

## ENM - eNanoMapper

Classified



Overview Browse DL Query Visualise PubMed Data SPARQL Download

label	zeta potential
oboid	NPO:1302
SubClassOf:	<a href="#">electric potential</a>
class	<a href="http://purl.bioontology.org/ontology/npo#NPO_1302">http://purl.bioontology.org/ontology/npo#NPO_1302</a>
<a href="http://purl.bioontology.org/ontology/npo#code">http://purl.bioontology.org/ontology/npo#code</a>	npo_1302
<a href="http://purl.bioontology.org/ontology/npo#dbXrefID">http://purl.bioontology.org/ontology/npo#dbXrefID</a>	ncit:C62354
<a href="http://purl.bioontology.org/ontology/npo#preferred_Name">http://purl.bioontology.org/ontology/npo#preferred_Name</a>	zeta potential
ontology	ENM
type	class

AberOWL is jointly developed by researchers from [King Abdullah University of Science and Technology](#), the [University of Birmingham](#), and the [University of Cambridge](#).

[Source code](#) [Issue tracker](#) [How to cite](#) [Help](#)

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# ENM in OLS

<http://www.ebi.ac.uk/ols/beta/ontologies/enm>

The screenshot displays the OLS interface for the ENM ontology. The breadcrumb trail is: OLS > eNanoMapper\_Ontology > ENM > NPO:1302. The term 'zeta potential' is selected, and its URI is shown as [http://purl.bioontology.org/ontology/npo#NPO\\_1302](http://purl.bioontology.org/ontology/npo#NPO_1302). A search bar labeled 'Search ENM' is present. The interface includes a tree view on the left showing the hierarchy: entity > disposition > electric potential > zeta potential. A 'Term info' panel on the right provides details for 'zeta potential':  
**code**: NPO\_1302  
**dBxrefID**: NCIT:C62354  
**preferred Name**: zeta potential  
A 'Term relations' panel below shows that 'zeta potential' is a subclass of 'electric potential'. Navigation options include 'Tree view', 'Term history', 'Graph view', and 'Show siblings'. A 'JSON' icon is visible in the top right corner of the main content area.





## Local browsing of eNM ontology



# Open from URL

<http://purl.enanomapper.org/onto/enanomapper.owl>

Or development version:

<http://purl.enanomapper.org/onto/enanomapper-dev.owl>





# ENM in Protégé

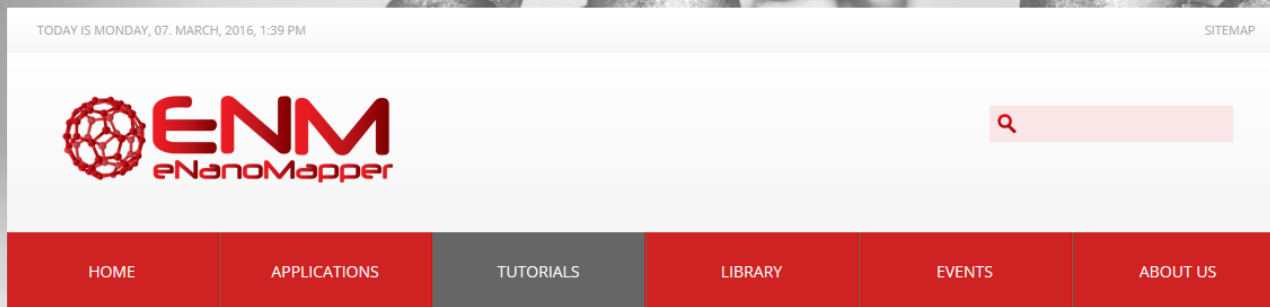
The screenshot displays the Protégé ontology editor interface. The main window shows the 'enanomapper' ontology. The left sidebar contains a class hierarchy tree under 'owl:Thing', with 'entity' expanded to show various subclasses, including 'zeta potential'. The main area is divided into several panes:

- Class hierarchy:** Shows the 'zeta potential' class selected.
- Annotations:** Lists properties and their values for 'zeta potential':
  - label [type: xsd:string]: zeta potential
  - code [type: xsd:string]: NPO\_1302 (with a note: **Asserted in: Optional of (http://purl.enanmapper.org/onto/external/npo-slim.owl)**)
  - dBXrefID [type: xsd:string]: NCIT:C62354
  - preferred\_Name [type: xsd:string]: zeta potential
- Description:** Shows the class 'zeta potential' and its relationships:
  - Equivalent To: (empty)
  - SubClass Of: 'electric potential'
  - General class axioms: (empty)
  - SubClass Of (Anonymous Ancestor): (empty)
  - Instances: (empty)
  - Target for Key: (empty)
  - Disjoint With: (empty)
  - Disjoint Union Of: (empty)



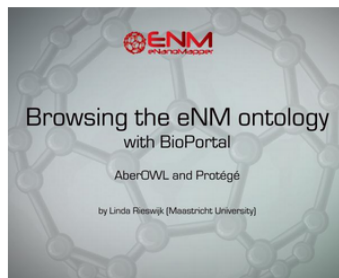
# Tutorial on browsing eNM ontology

[enanomapper.net/enm-tutorials](http://enanomapper.net/enm-tutorials)



The screenshot shows the top section of the eNanoMapper website. At the top left, it says "TODAY IS MONDAY, 07. MARCH, 2016, 1:39 PM". At the top right, there is a "SITEMAP" link. The main header features the eNM logo (a red sphere with a molecular structure) and the text "eNanoMapper". To the right of the logo is a search bar with a magnifying glass icon. Below the header is a navigation menu with six items: HOME, APPLICATIONS, TUTORIALS, LIBRARY, EVENTS, and ABOUT US. The "TUTORIALS" item is highlighted with a dark grey background.

## TUTORIALS



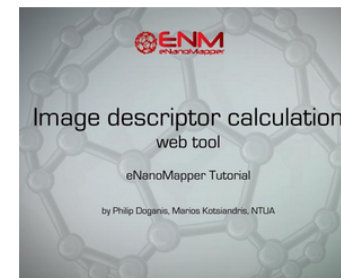
The card features the eNM logo at the top. The main text reads "Browsing the eNM ontology with BioPortal" and "AberOWL and Protégé". Below that, it says "by Linda Reeswijk (Maastricht University)". The background is a light grey molecular structure.

**BROWSING THE ONTOLOGY**  
Browsing the eNM ontology with BioPortal, AberOWL...



The card features the eNM logo at the top. The main text reads "Enriching protein corona fingerprints" and "An integration technique". Below that, it says "by Georgia Tsiiliki (NTUA, Greece)". The background is a light grey molecular structure.

**ENRICHING PROTEIN CORONA**  
Enriching protein corona fingerprints using gene...



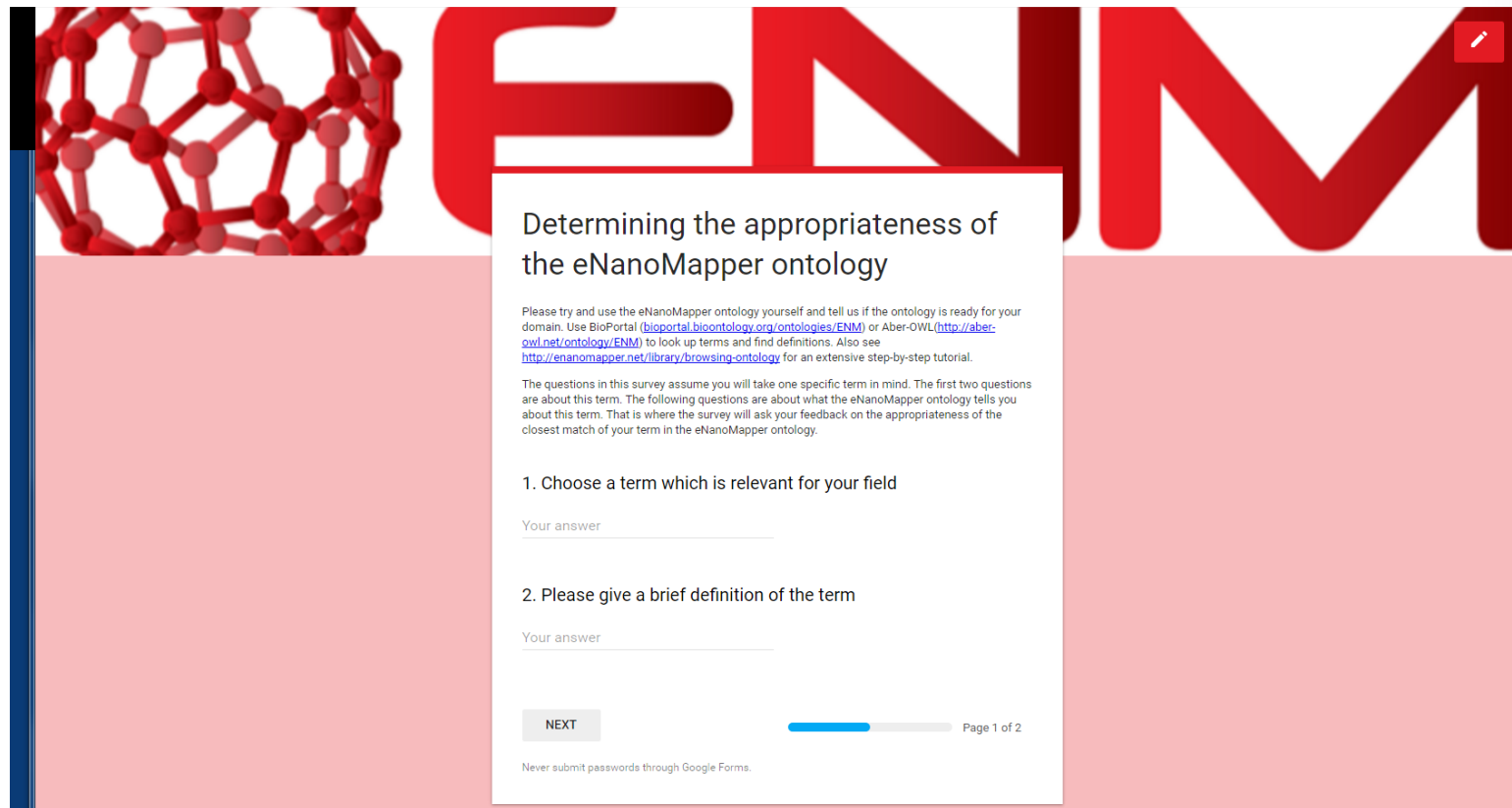
The card features the eNM logo at the top. The main text reads "Image descriptor calculation web tool" and "eNanoMapper Tutorial". Below that, it says "by Philip Dogaenis, Manos Kotsandris, NTUA". The background is a light grey molecular structure.

**IMAGE DESCRIPTOR TUTORIAL**  
Image descriptor calculation web tool Authors:...



# Evaluation of the eNM ontology

<https://docs.google.com/forms/d/e/1FAIpQLScYMQWy4ULxmK7tyU4NCNPocnQNEiQw9c62eneAQP7vll3tSg/viewform>



**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](http://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

Your answer

2. Please give a brief definition of the term

Your answer

**NEXT** Page 1 of 2

Never submit passwords through Google Forms.

# Requests for additions available via Issue Tracker on GitHub

<https://github.com/enanomapper/ontologies/issues>

Personal Open source Business Explore Pricing Blog Support This repository Search Sign in Sign up

enanomapper / ontologies Watch 14 Star 2 Fork 5

Code Issues 20 Pull requests 0 Projects 0 Wiki Pulse Graphs

is:issue is:open Labels Milestones New issue

20 Open 73 Closed Author Labels Milestones Assignee Sort

- nanoparticle classes need to be re-located #96 opened 2 days ago by JKChang2015 1
- ENMRDF uses several predicates that should be available in the ENM ontology #94 opened 5 days ago by egonw 0 of 2
- We need to make more evident the difference among Zeta potential entries #86 opened on 24 Oct by dphilip 3
- language tag for labels enhancement #84 opened on 24 Oct by gebele 1
- New release of NANoREG templates - assay list enhancement #82 opened on 10 Oct by vedina 2
- Terms from NANoREG harmonised terminology enhancement #77 opened on 26 Sep by vedina 1
- High-throughput screening and high content analysis related ontologies #76 opened on 20 Sep by pennym
- Bioinformatics ontology #75 opened on 20 Sep by pennym 1
- Functionality-related terminology being developed in NanoREG2 enhancement #74 opened on 20 Sep by pennym
- "endpoint measured by assay" statements #73 opened on 7 Sep by vedina 6
- Terms from NanoReg templates ENM #66 opened on 6 Jun by vedina 4
- Not all terms have descriptions bug

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# Usability of the eNM Ontology

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# Data completeness according to reporting and curation standards

## Minimal Reporting Standards provided by:

- Nanomaterial Data Curation Initiative (NDCI)
- Uniform Description System (UDS) by CODATA/VAMAS Joint Working Group
- Nanomaterial Registry (Minimal Information about Nanomaterials (MIAN))



# Nanomaterial Registry

Physico-chemical characteristics	
PPCs MIAN standards	eNM ontology entity URIs
Aggregation	<a href="http://purl.bioontology.org/ontology/npo#NPO_1967">http://purl.bioontology.org/ontology/npo#NPO_1967</a>
Shape	<a href="http://purl.bioontology.org/ontology/npo#NPO_274">http://purl.bioontology.org/ontology/npo#NPO_274</a>
Particle size	<a href="http://purl.bioontology.org/ontology/npo#NPO_1694">http://purl.bioontology.org/ontology/npo#NPO_1694</a>
Size distribution	<a href="http://purl.bioontology.org/ontology/npo#NPO_1697">http://purl.bioontology.org/ontology/npo#NPO_1697</a>
Surface area	<a href="http://purl.bioontology.org/ontology/npo#NPO_1235">http://purl.bioontology.org/ontology/npo#NPO_1235</a>
Composition	<a href="http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C53414">http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C53414</a>
Surface charge	<a href="http://purl.bioontology.org/ontology/npo#NPO_1812">http://purl.bioontology.org/ontology/npo#NPO_1812</a>
Surface reactivity	-
Stability	<a href="http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C54072">http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C54072</a>
Solubility	<a href="http://purl.obolibrary.org/obo/PATO_0001536">http://purl.obolibrary.org/obo/PATO_0001536</a>
Surface chemistry	<a href="http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C64351">http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C64351</a>
Purity	<a href="http://purl.obolibrary.org/obo/UO_0000193">http://purl.obolibrary.org/obo/UO_0000193</a>



# Data searching using SPARQL queries

Availability of 'Particle size' (*NPO\_1694*) for some nanomaterial (NWKI-002f5129-d46a-39c7-8f26-5626aec2174e) using the SPARQL query:

```
prefix obo: <http://purl.obolibrary.org/obo/>
prefix bao: <http://www.bioassayontology.org/bao#>
prefix sso: <http://semanticscience.org/resource/>
prefix npo: <http://purl.bioontology.org/ontology/npo#>
prefix ex: <http://localhost/ambit2/substance/>
```

```
select distinct ?substance ?type ?title ?value ?unit where {
  BIND (ex:NWKI-002f5129-d46a-39c7-8f26-5626aec2174e as ?substance)
  BIND (npo:NPO_1694 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 for data completeness

The script tests for the availability of data for nine properties: NPO\_1967, NPO\_274, NPO\_1694, NPO\_1697, NPO\_1235, NPO\_1812, and NPO\_1302 from the NanoParticle Ontology, and these two from other ontologies: PATO\_0001536, and C53414

An HTML report is generated reporting the properties found and an indication of which are missing (left side). A score is generated for all PhysChem properties to represent the data completeness.

<b>Fe3O4 MION-47 no. 35</b>				
<a href="#">Open in eNanoMapper</a>				
<b>Particle size</b>				
type	title	assaySpec	value range	unit
npo:NPO_1694	Primary Particle Size		20.0	nm
<b>Zeta potential</b>				
type	title	assaySpec	value range	unit
npo:NPO_1302	Zeta Potential		-13.6	mV
<b>Composition</b>				
type	name	smiles		
npo:NPO_1617	Fe3O4	<chem>O=[Fe].O=[Fe]O[Fe]=O</chem>		
npo:NPO_1367	Dextran			
Score: 46 %				
Missing data for: Aggregation Shape Size distribution Surface area Surface charge Solubility				

# Incorporated in search functionality of eNM database

The screenshot shows the eNanoMapper search interface. The browser address bar displays <https://search.data.enanmapper.net>. The navigation menu includes Home, Search, Data collections, Data upload, Data templates, For developers, and Help. The main content area features a search bar with the query 'NPO\_']' and a 'Feedback' link. Below the search bar, a dropdown menu lists various identifiers: NPO\_112 (5) - substanceType, c9npo\_112 (5) - \_text\_, npo\_112 (5) - \_text\_, npo\_126 (5) - \_text\_, npo\_1417 (2) - \_text\_, npo\_1436 (2) - \_text\_, npo\_1441 (1) - \_text\_, npo\_1465 (1) - \_text\_, npo\_1469 (1) - \_text\_, npo\_1487 (5) - \_text\_, npo\_1539 (1) - \_text\_, npo\_1895 (1) - \_text\_, and npo\_2000 (2) - \_text\_.

On the left side, there is a sidebar with a 'Data sources (3)' section and a 'Nanomaterial type (5)' section. The 'Nanomaterial type (5)' section is expanded to show 'multi-walled nan...'. Below this, there are buttons for 'P-CHEM (2)', 'TOX (3)', 'Cell (3)', 'Species (0)', 'Results (0)', 'References (3)', 'Protocols (3)', and 'Instruments (0)'. The main search results area is titled 'Hits list' and 'Selection'. It shows a search filter 'multi-walled nanotube' and indicates 'displaying 1 to 5 of 5' results. The results are as follows:

- NIOSH-VWalkerTAP2009-03 multi-walled nanotube**  
P-CHEM.Particle size distribution (Granulometry) [more](#)  
[caNanoLab](#)
- KI-HKarlssonCRT2008-08 multi-walled nanotube**  
P-CHEM.Particle size distribution (Granulometry) well with the particle size in the different nanopowder [more](#)  
[caNanoLab](#)
- SNU-NJiaNL2007-01 multi-walled nanotube**  
P-CHEM.Particle size distribution (Granulometry) [\[2007\]](#) [more](#)  
[caNanoLab](#)
- SNU-NJiaNL2007-02 multi-walled nanotube**



# Conclusions and future perspectives

- Many SPARQL queries are required to cover all MIAN
- PhysChem data missing from literature
- Data lacking ontological annotation
- To be continued in collaboration with the caLIBRAte project (focussed on development of parameter criteria for risk assessment tools → SPARQL queries for finding specific data)



# Further information

- Hastings, J., Jeliaskova, N., Owen, G., Tsiliki, G., Munteanu, C.R., Steinbeck, C., and Willighagen, E. (2015) eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment. *Journal of Biomedical Semantics*, 6, 10.(doi:10.1186/s13326-015-0005-5);
- The eNanoMapper ontology in BioPortal (<http://bioportal.bioontology.org/ontologies/ENM>);
- The eNanoMapper ontology in AberOWL (<http://aber-owl.net/ontology/ENM>);
- Slimmer version of external re-used ontologies present in eNanoMapper ontology within GitHub (<https://github.com/enanomapper/ontologies>);
- Open-source ontology editor Protégé (<http://protege.stanford.edu/>);
- The eNanoMapper ontology OWL within GitHub (<https://github.com/enanomapper/ontologies>);
- eNanoMapper Issue Tracker within GitHub (<https://github.com/enanomapper/ontologies/issues>);
- eNanoMapper Pull Requests within GitHub (<https://github.com/enanomapper/slimmer/pulls>);
- Whetzel, P.L., Noy, N.F., Shah, N.H., Alexander, P.R., Nyulas, C., Tudorache, T., and Musen, M.A. (2011) BioPortal: enhanced functionality via new Web services from the National Center for Biomedical Ontology to access and use ontologies in software applications. *Nucleic Acids Res*, 39, W541-545 (doi: 10.1093/nar/gkr469);
- Hoehndorf, R., Slater, L., Schofield, P.N., and Gkoutos, G.V. (2015) Aber-OWL: a framework for ontology-based data access in biology. *BMC Bioinformatics*, 16, 1-9 (doi:10.1186/s12859-015-0456-9);
- Tutorial for browsing the eNanoMapper Ontology <http://enanomapper.net/library/browsing-ontology>.



# Acknowledgements



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