The eNanoMapper Ontology

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What is an ontology and why do we use it?

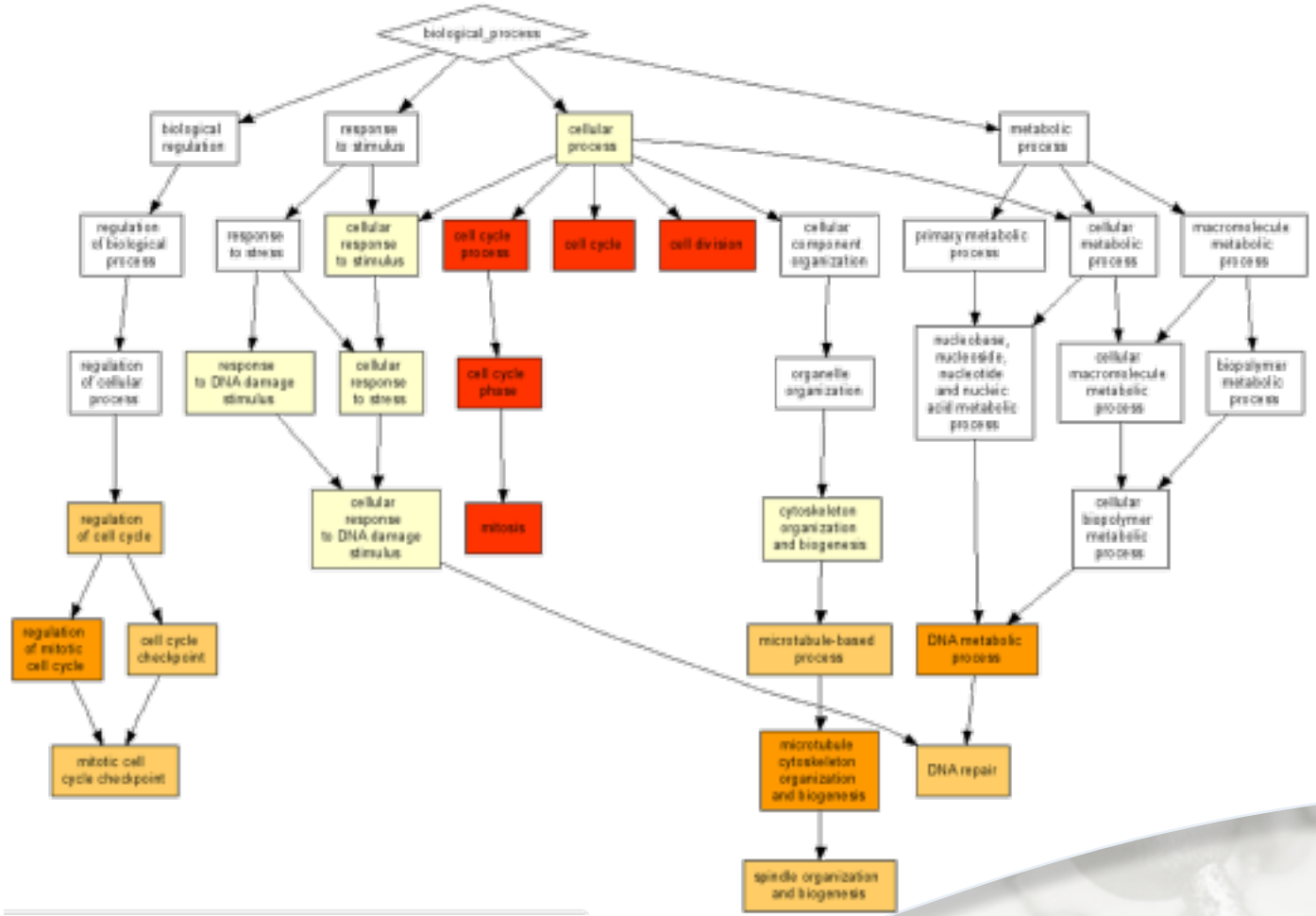
Definition:

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

Usage:

- Harmonize data
- Federated SPARQL queries

THE example : GENEONTOLOGY



eNanoMapper

Development of eNanoMapper (ENM) ontology

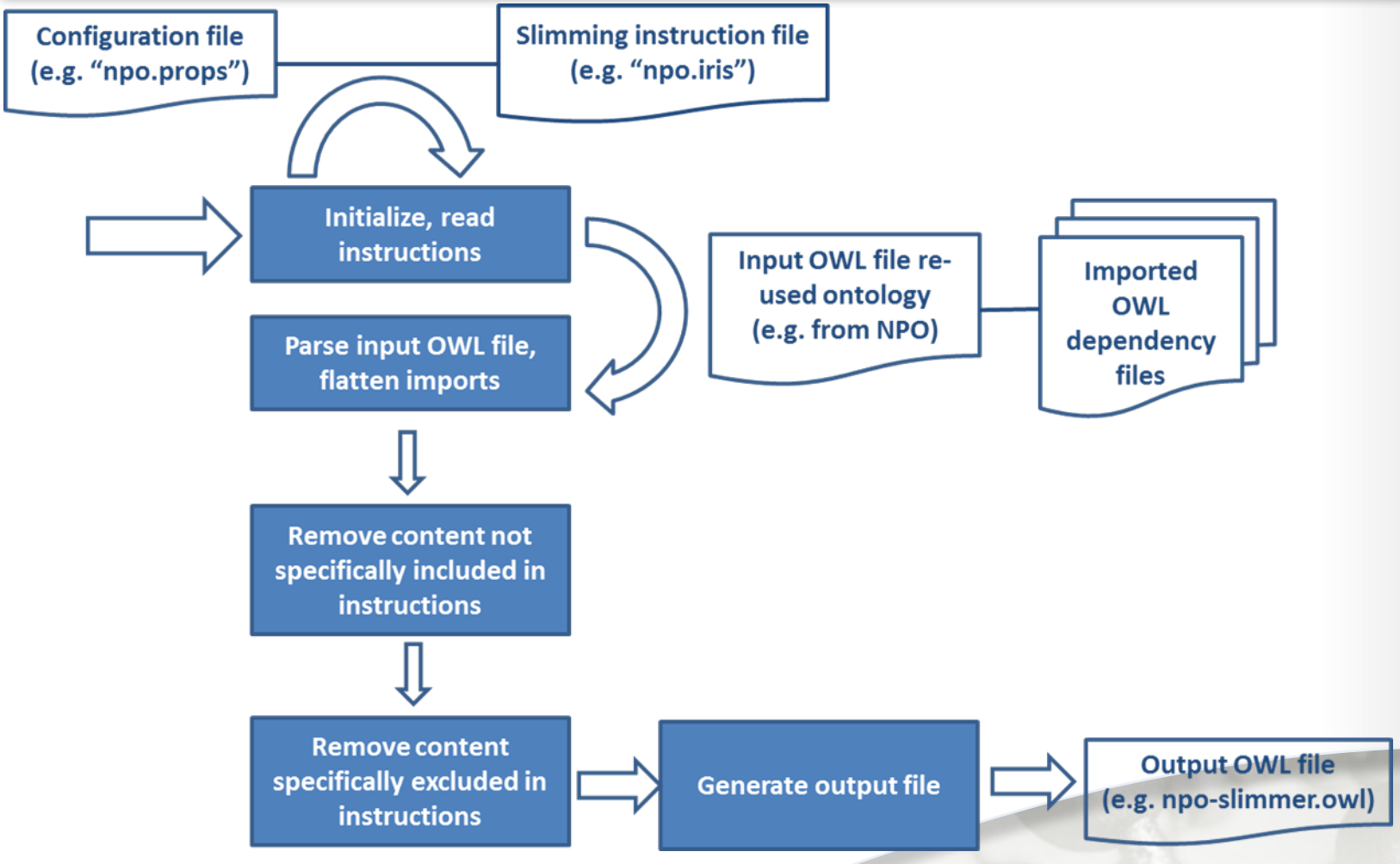
- Why reuse?
  - Annotations in existing ontologies reused
  - Integration of fragmented annotations ≠ possible
  - Do not reinvent the wheel
  - Feedback to original external ontologies

Reused external ontologies

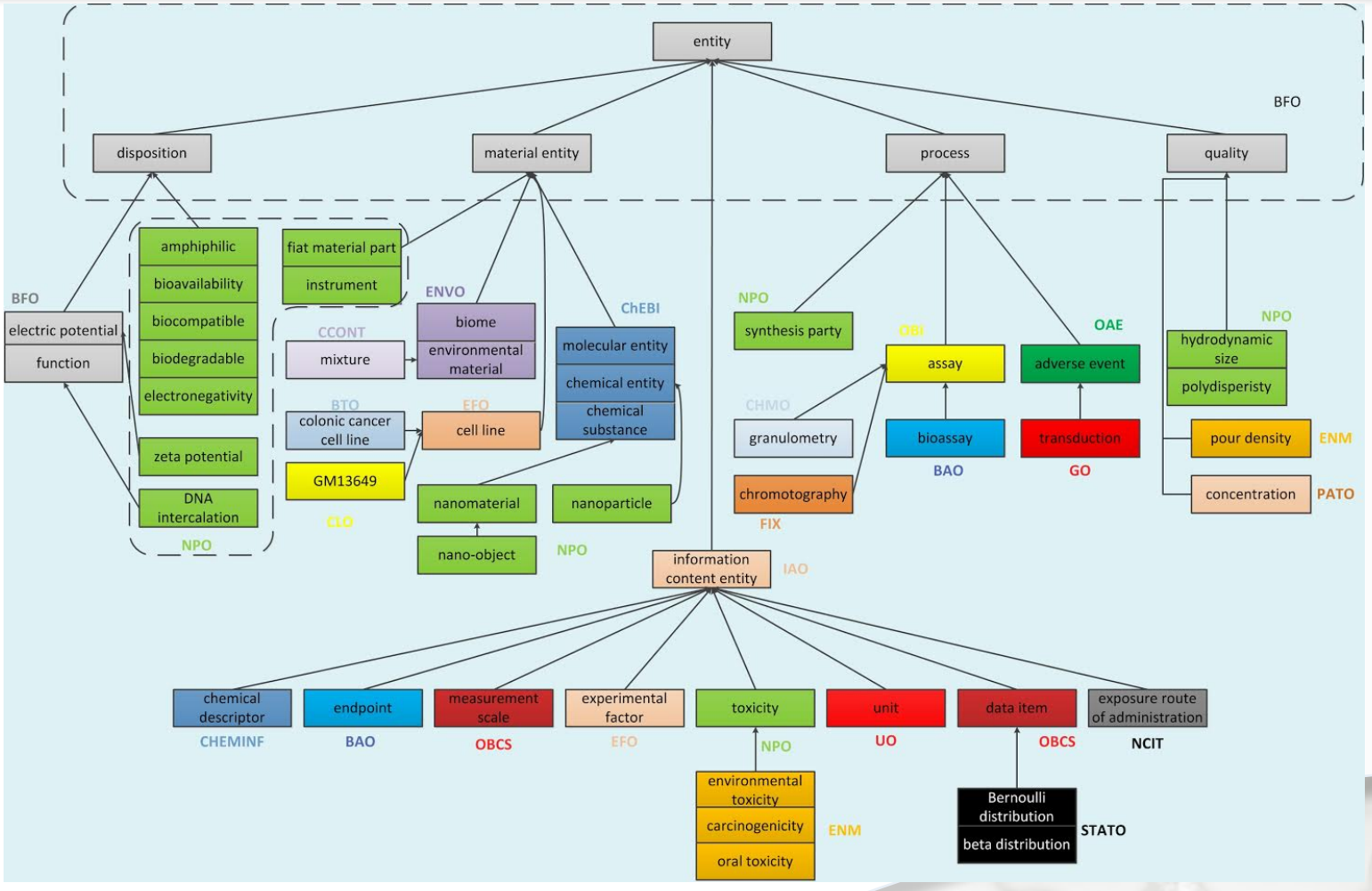
Version 3 of the eNM ontology contains 21 external ontology sources

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		

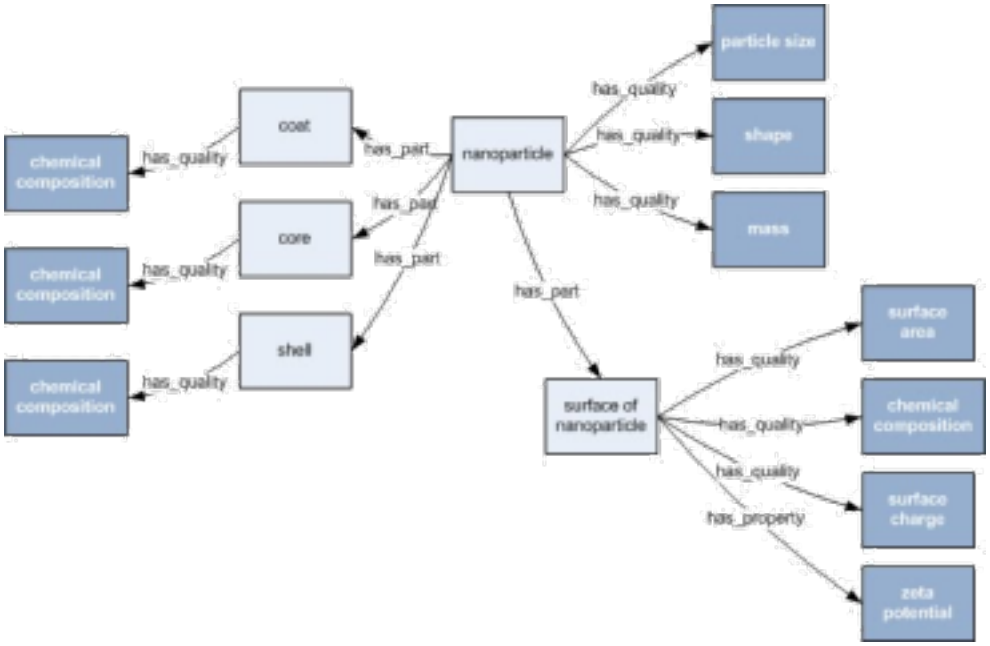
Slimming procedure – “Only grab what is necessary”



eNanoMapper Ontology v.3.



Re-use of NanoParticle Ontology (NPO)



Browsing the eNanoMapper Ontology

Online:

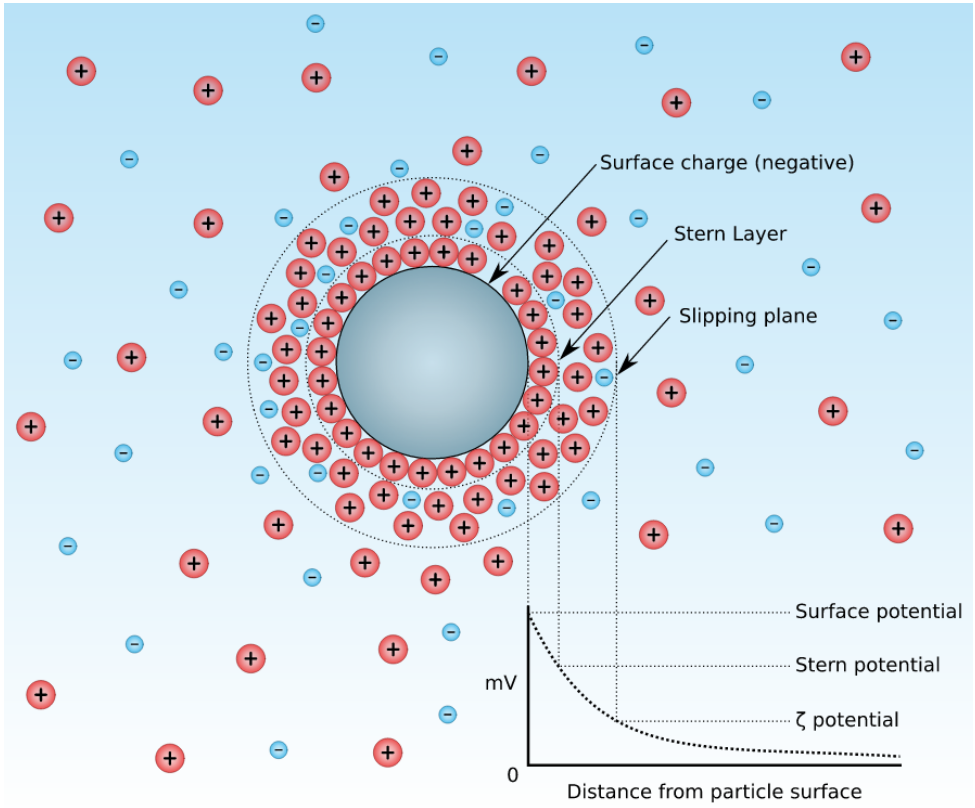
Three main ontology repositories:

- –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



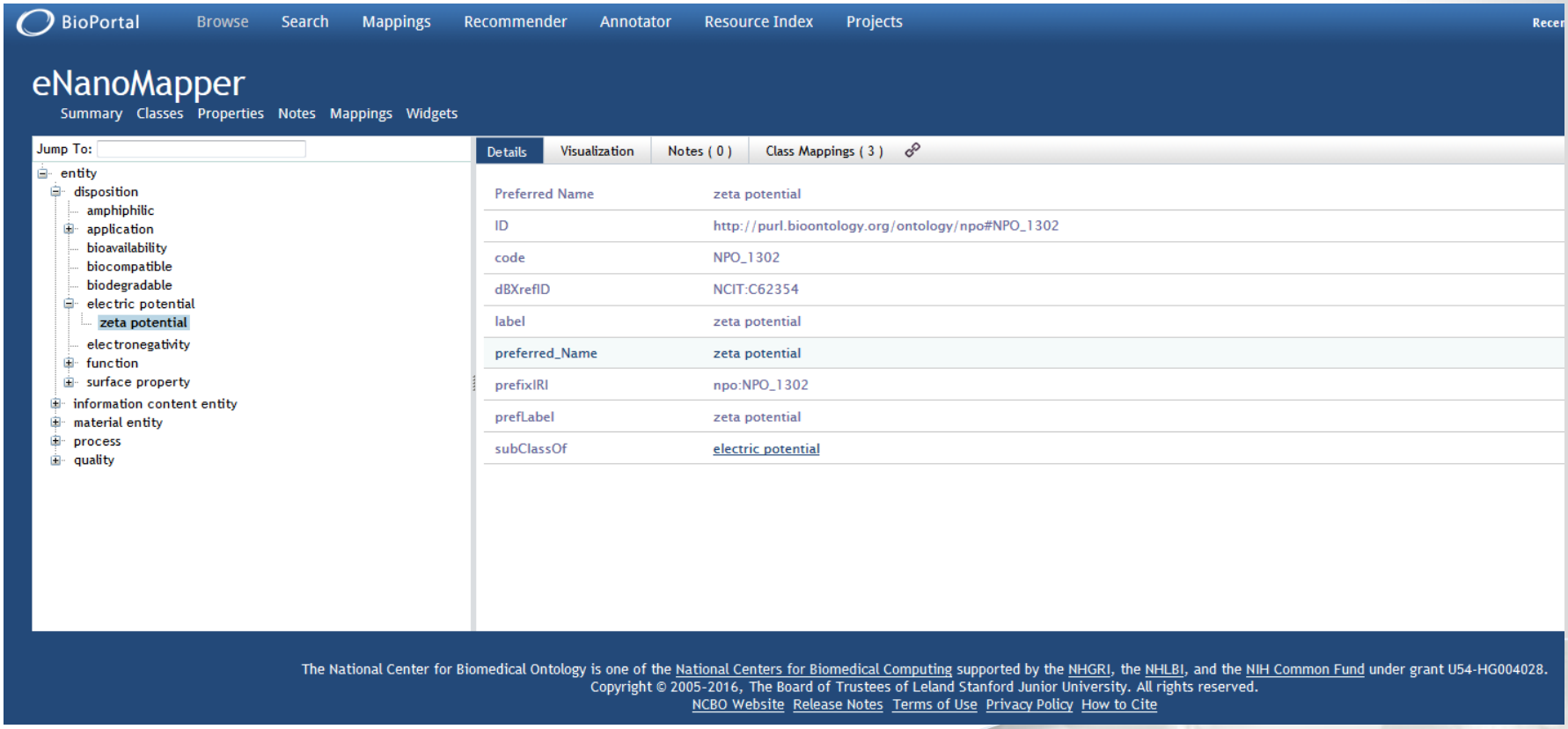
Definition:

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

Online browsing of eNM ontology

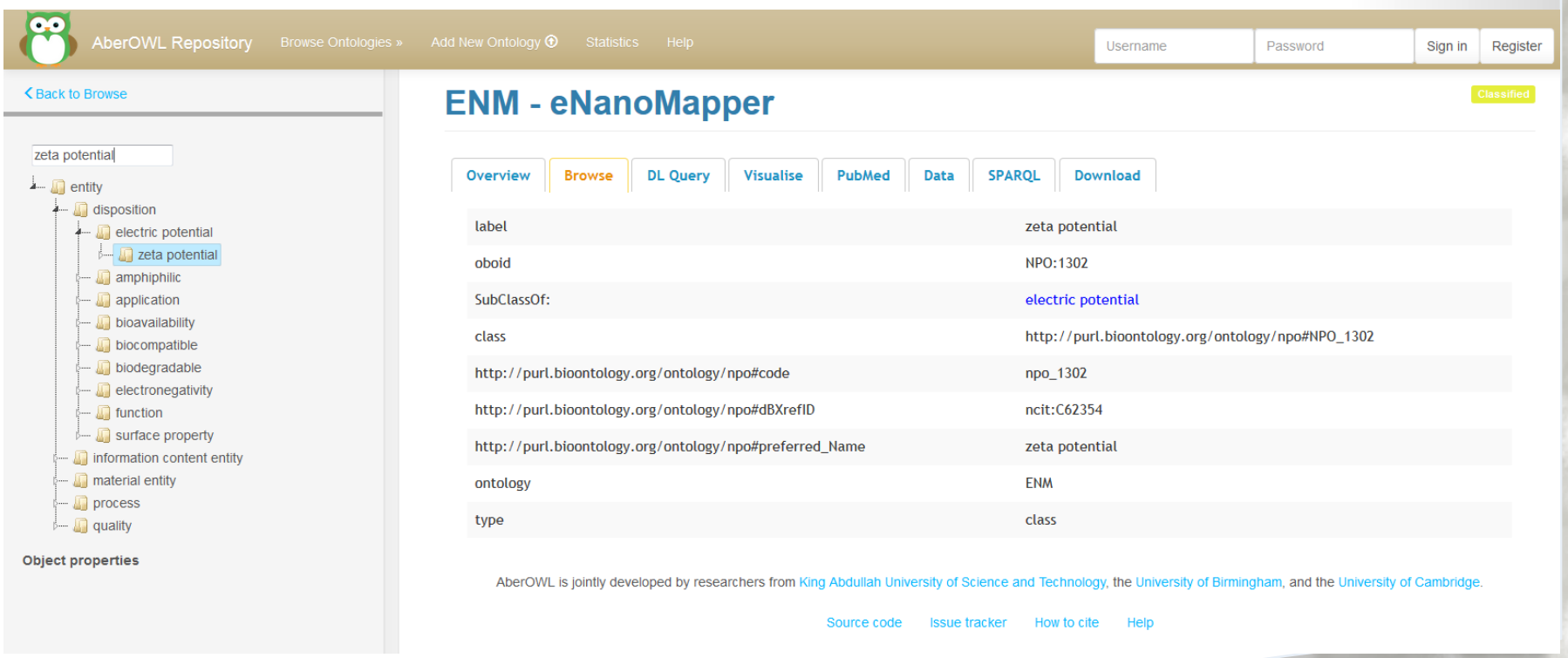
ENM in BioPortal

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



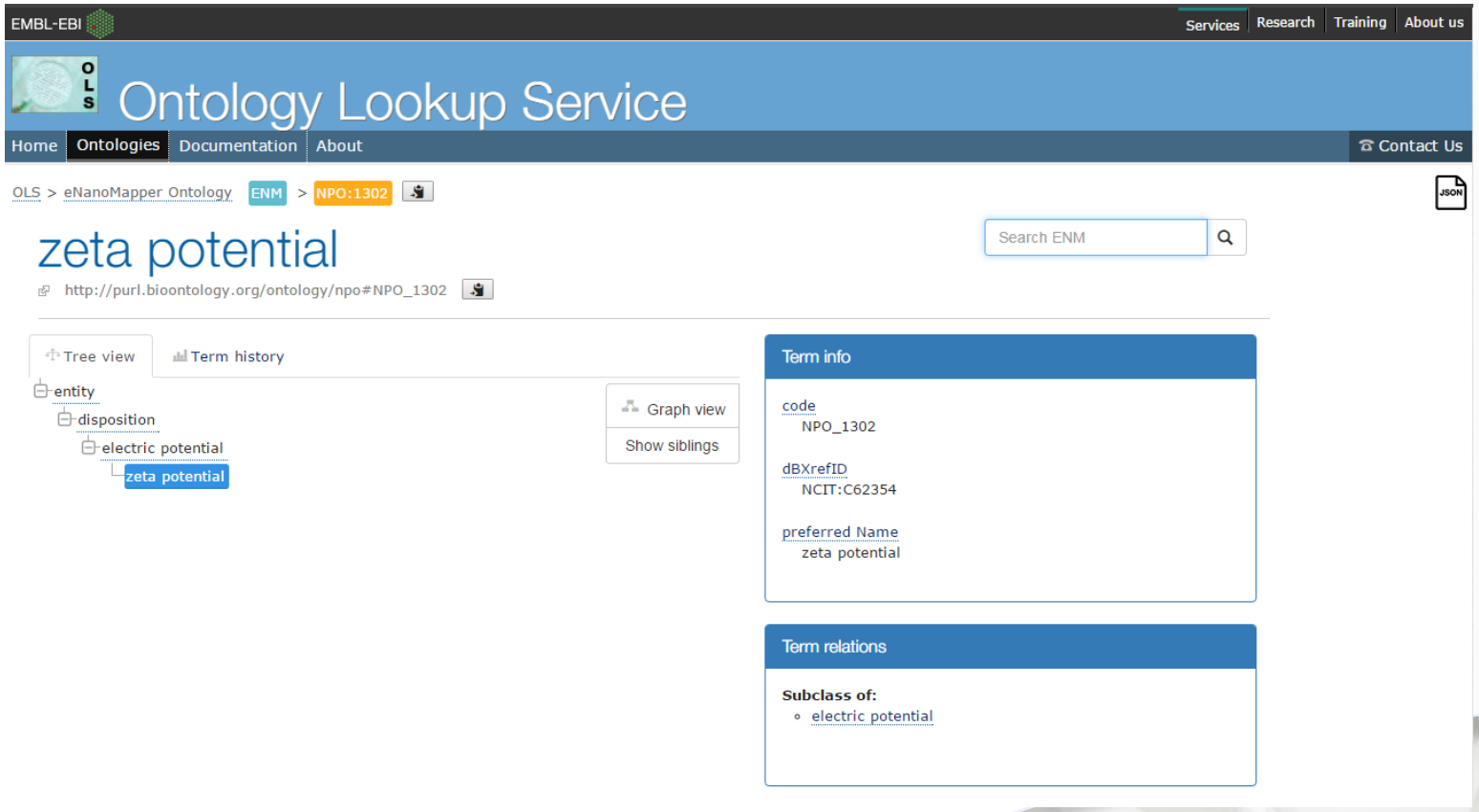
ENM in Aber-OWL

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



ENM in OLS

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



Local browsing of eNM ontology

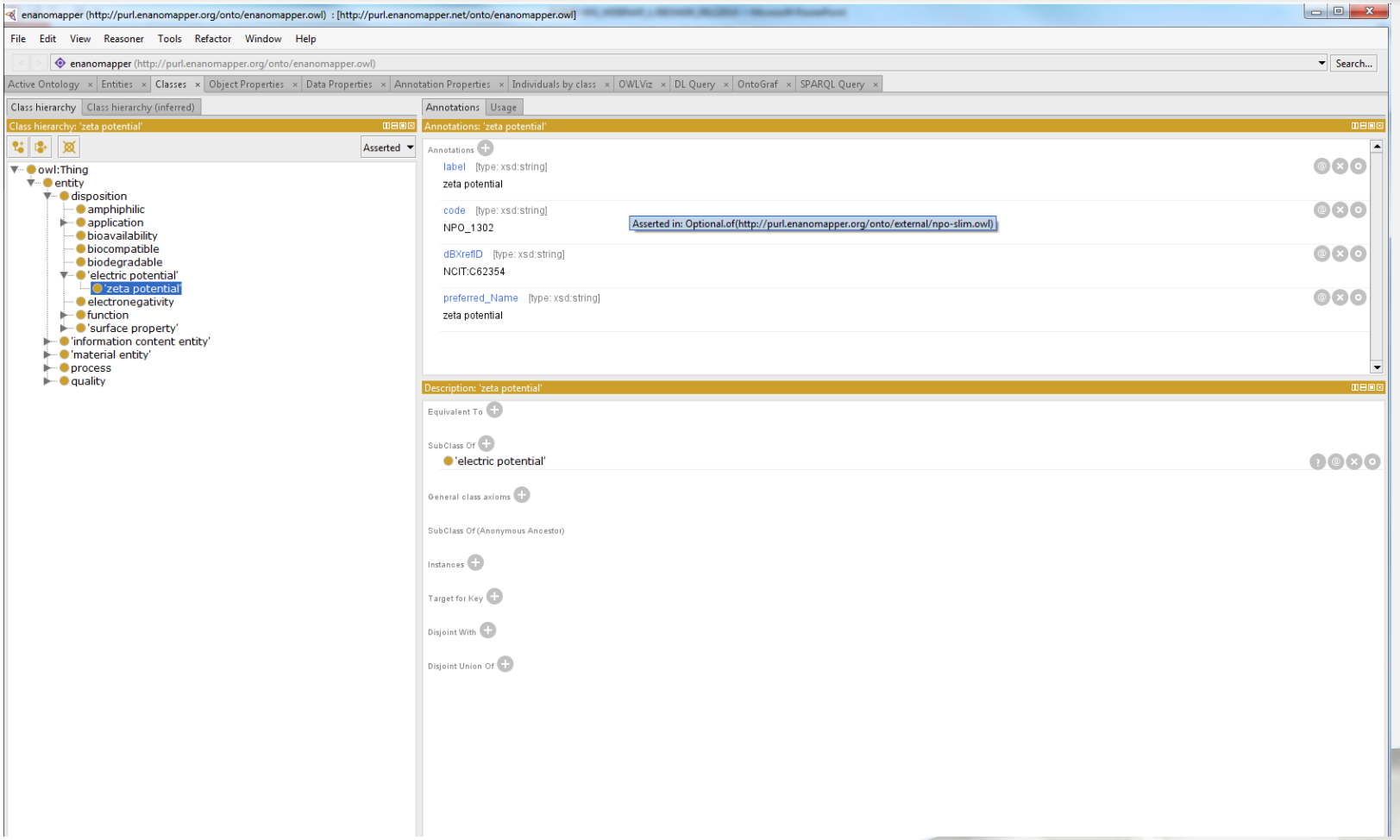
Open from URL

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

Or development version:

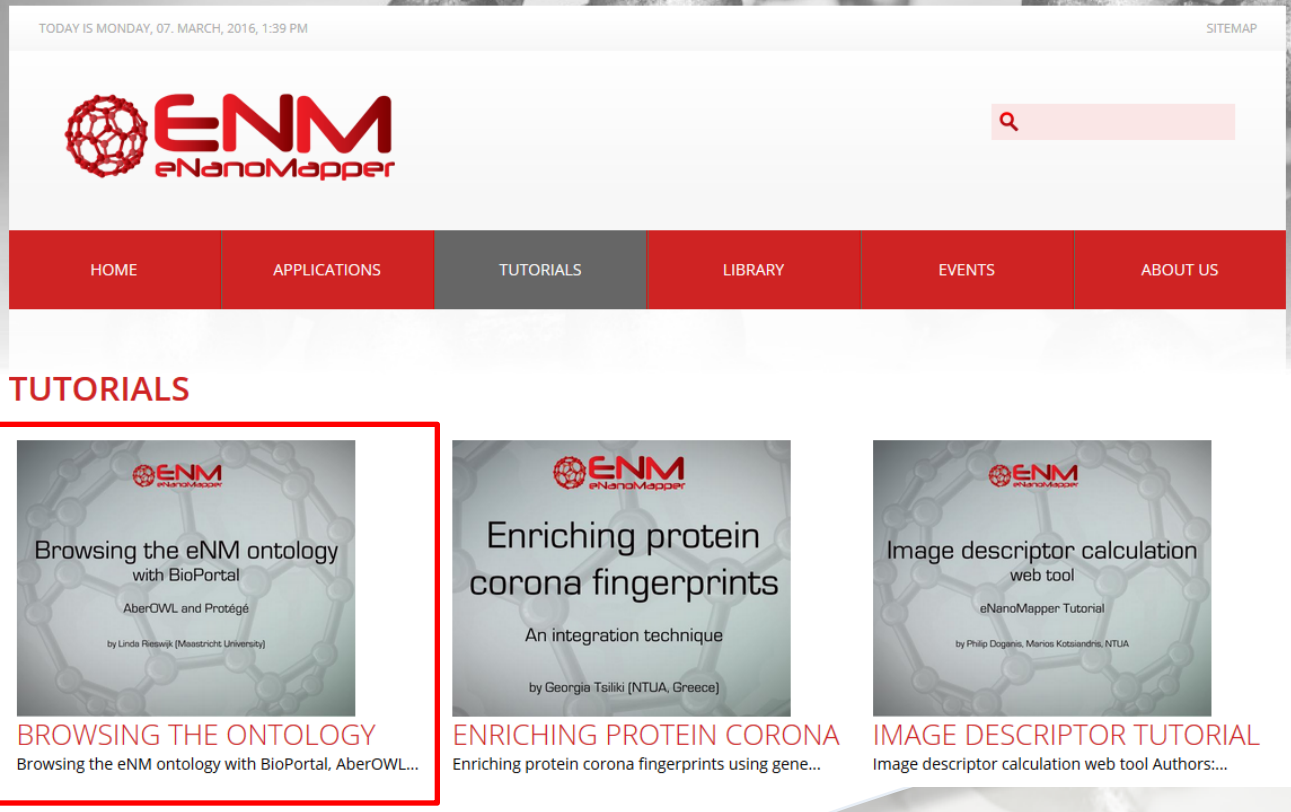
http://purl.enanomapper.org/onto/enanomapper-dev.owl

ENM in Protégé



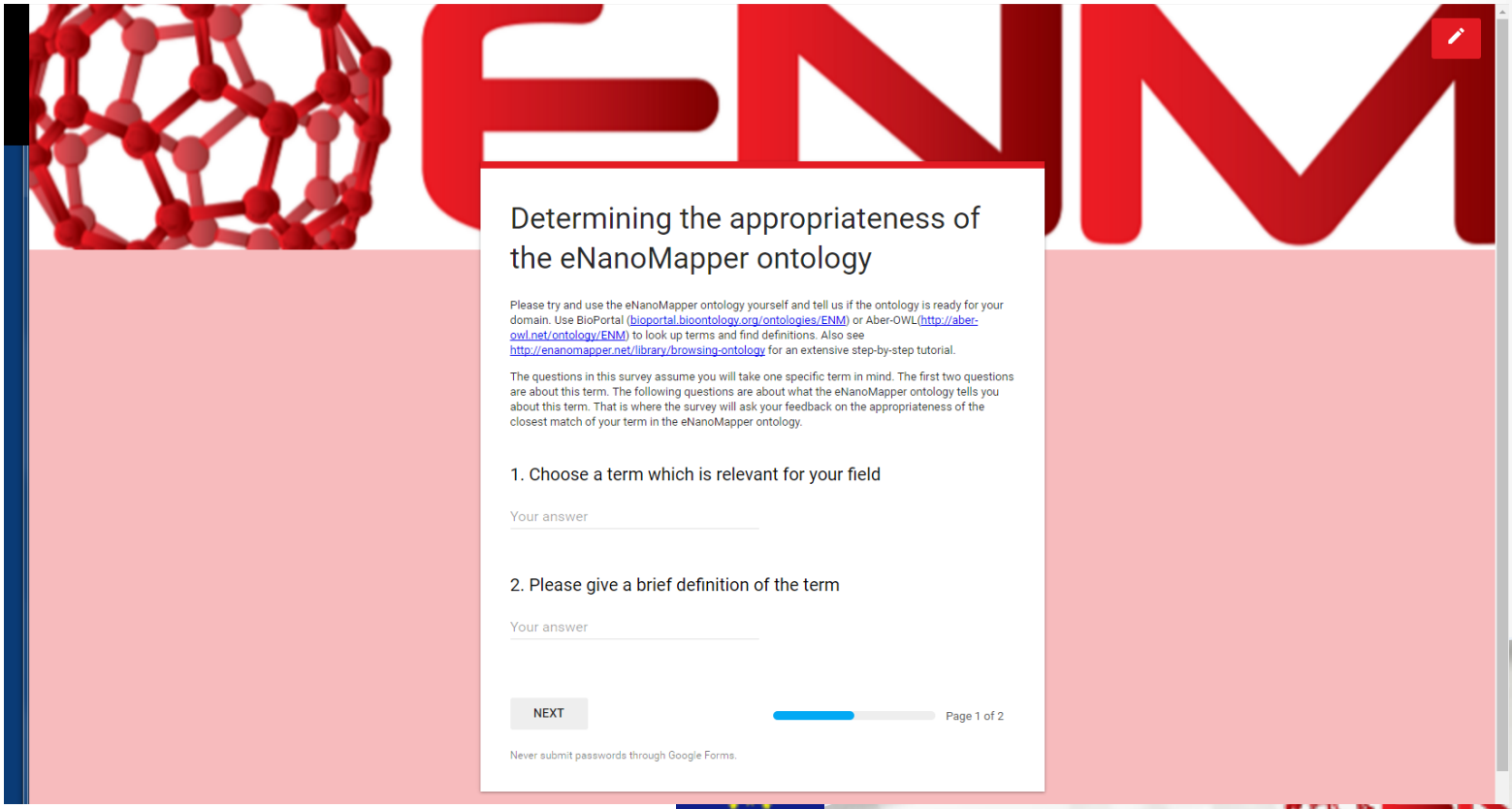
Tutorial on browsing eNM ontology

enanomapper.net/enm-tutorials



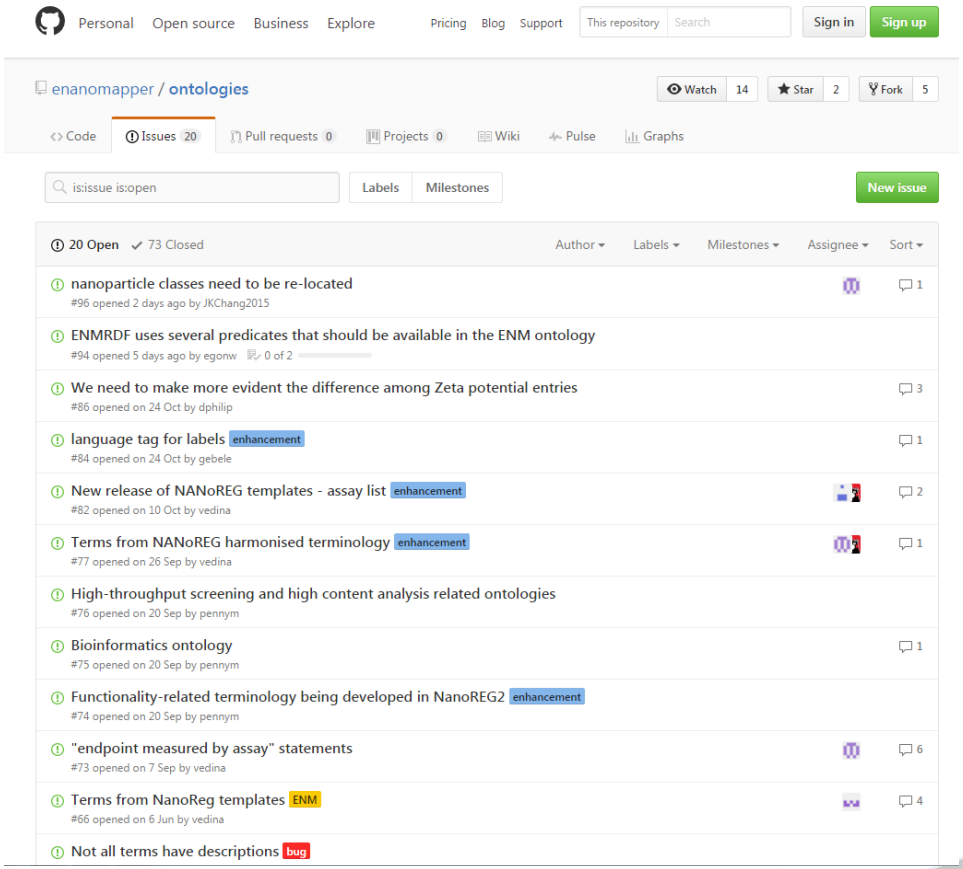
Evaluation of the eNM ontology

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



Requests for additions available via Issue Tracker on GitHub

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



Usability of the eNM Ontology

8 December 2016

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	http://purl.bioontology.org/ontology/npo#NPO_1967
Shape	http://purl.bioontology.org/ontology/npo#NPO_274
Particle size	http://purl.bioontology.org/ontology/npo#NPO_1694
Size distribution	http://purl.bioontology.org/ontology/npo#NPO_1697
Surface area	http://purl.bioontology.org/ontology/npo#NPO_1235
Composition	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C53414
Surface charge	http://purl.bioontology.org/ontology/npo#NPO_1812
Surface reactivity	-
Stability	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C54072
Solubility	http://purl.obolibrary.org/obo/PATO_0001536
Surface chemistry	http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C64351
Purity	http://purl.obolibrary.org/obo/UO_0000193

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)
```

eNM eNanoMapper

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.

Fe3O4 MION-47 no. 35

Open in eNanoMapper

Particle size

type	title	assaySpec	value	range	unit
npo:NPO_1694	Primary Particle Size		20.0		nm

Zeta potential

type	title	assaySpec	value	range	unit
npo:NPO_1302	Zeta Potential		-13.6		mV

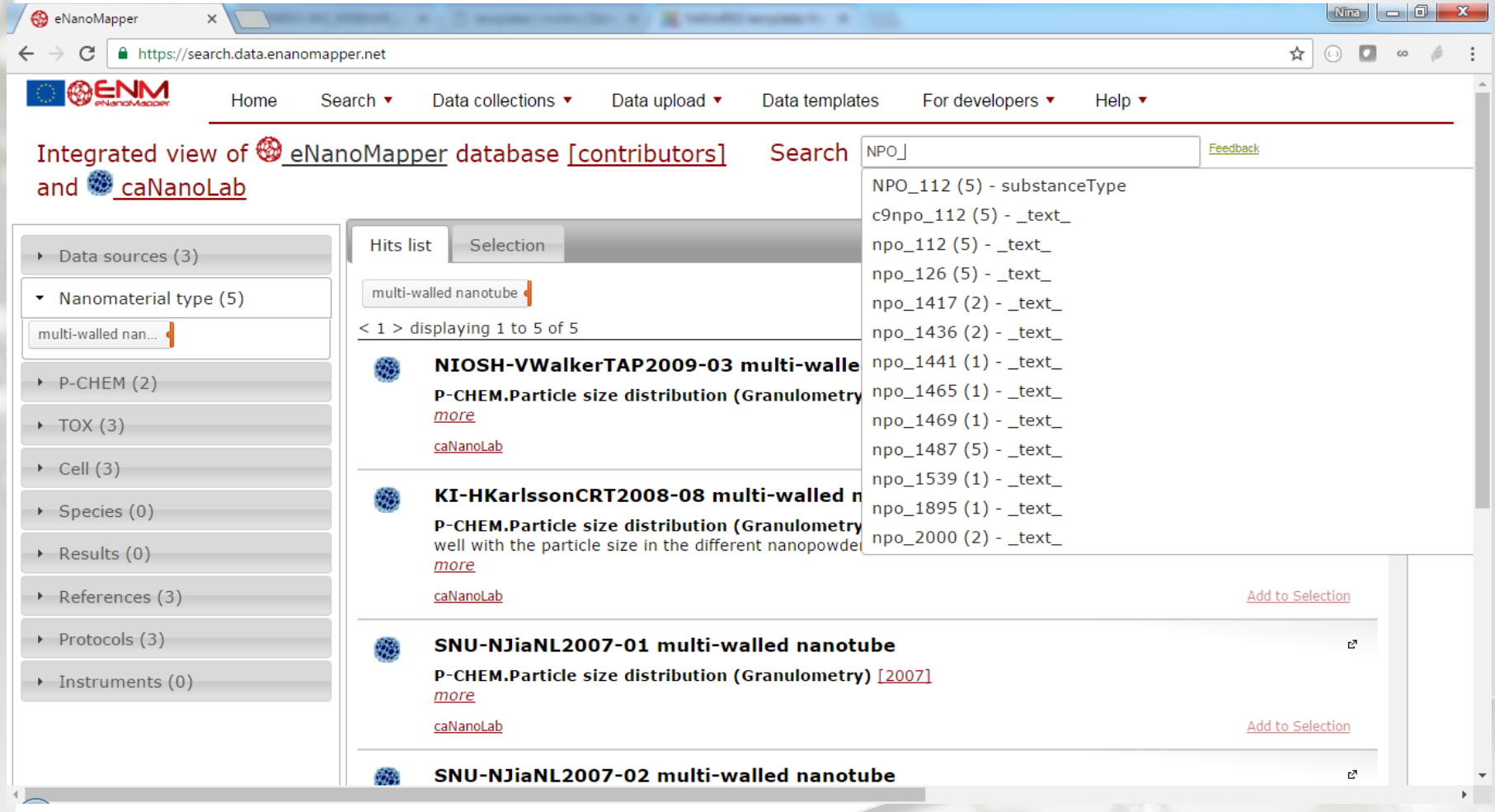
Composition

type	name	smiles
npo:NPO_1617	Fe3O4	O=[Fe].O=[Fe]O[Fe]=O
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



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., Jeliazkova, 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

eNanoMapper