

Using the eNanoMapper ontology

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www.enanomapper.net



Overview

- Ontology re-use pipeline
- Ontology structure and content
- Using the ontology: BioPortal
- Using the ontology: Protégé
- Requesting additional terms: GitHub
- Ongoing and future work

RE-USE PIPELINE

Ontology development through reuse

- NanoParticle Ontology (NPO)
 - Chemical Entities of Biological Interest (ChEBI)
 - Chemical Information Ontology (CHEMINF)
 - Ontology for Biomedical Investigations (OBI)
 - BioAssay Ontology (BAO)
 - Environment Ontology (ENVO)
AND OTHERS
- + Editing using OWL and Protégé

Technical Strategy

- Split up source ontologies into “minimal units” for each different part of the domain covered
- Sort out duplication by removing entities from one of the ontologies’ relevant modules (e.g. removing groups from NPO, removing nanoparticle classification from ChEBI)
- Import these minimal units back into a fully assembled ontology
- Automated so that it can be done over and over with source ontology releases

“Slimmer” library on GitHub

enanomapper / **slimmer** Unwatch ▾ 6

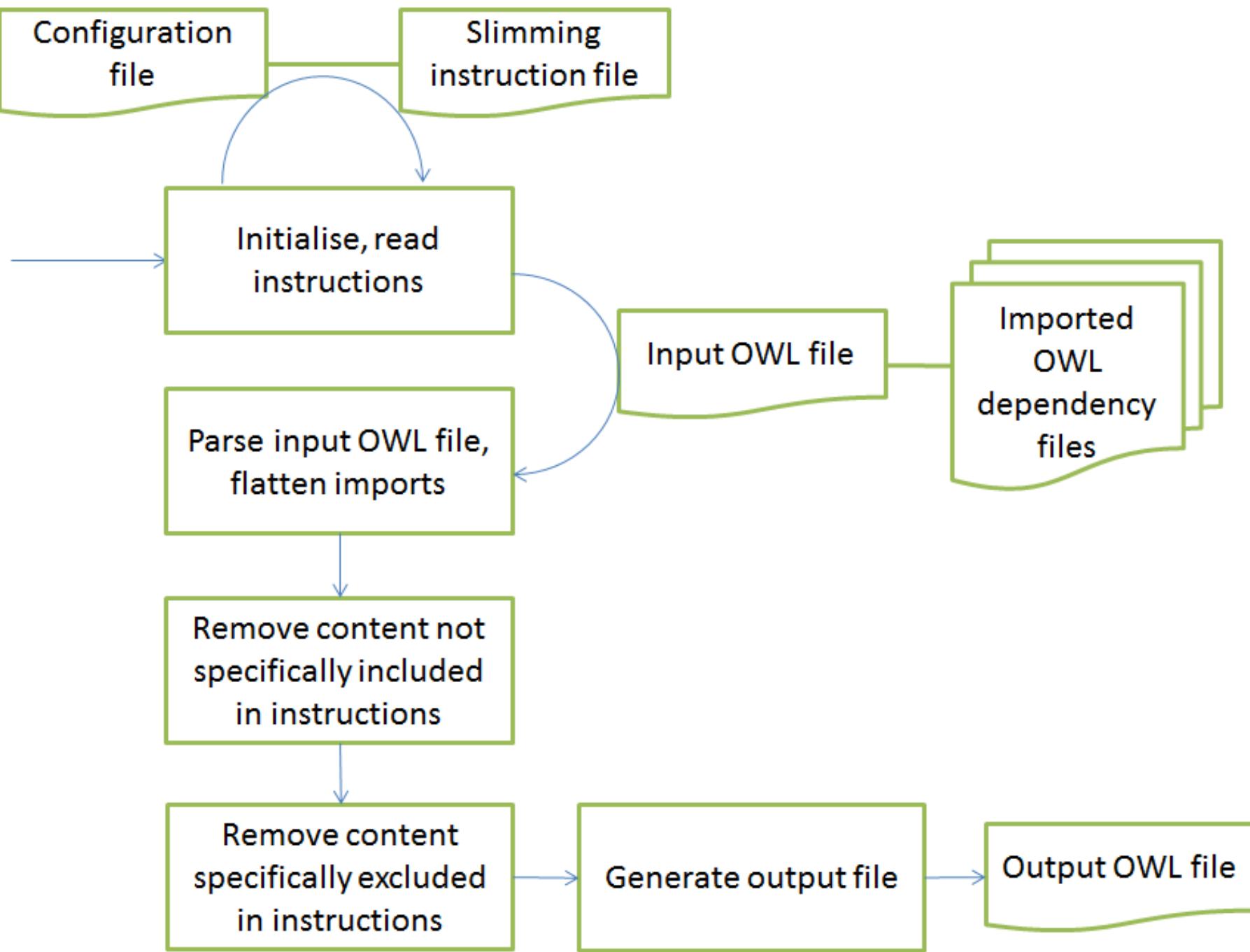
Slims ontologies. — Edit

112 commits 1 branch 0 releases 2 contributors

branch: master **slimmer** / +

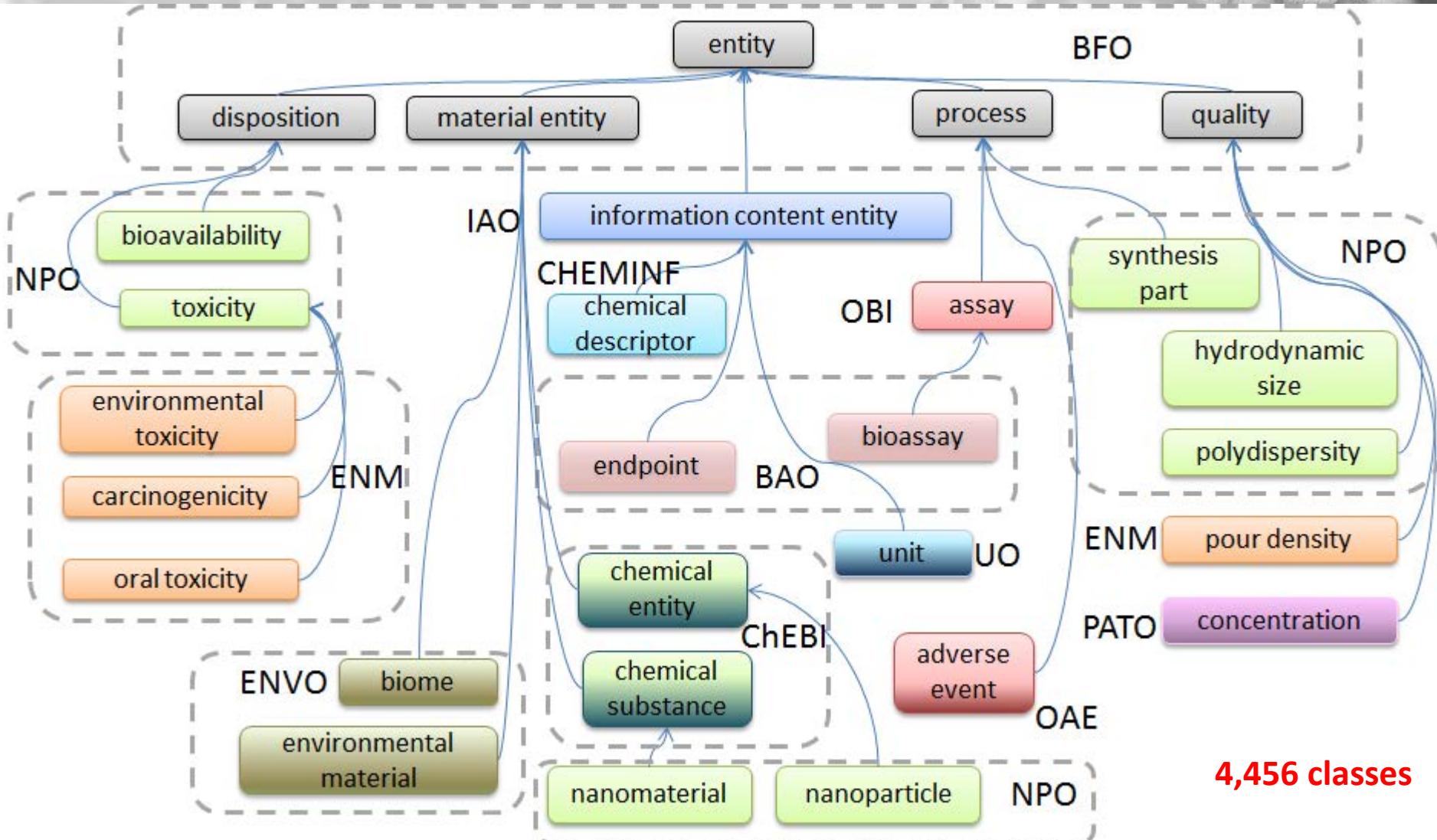
Update npo.iris ...

	jannahastings authored 6 days ago	latest commit 1b7f0f2e97
	src Update npo.iris	6 days ago
	.gitignore It can now read an ontology	4 months ago
	.project Found the culprit	4 months ago
	LICENSE Create LICENSE	2 months ago
	README.md Added more detail about how Slimmer works.	9 days ago
	pom.xml Added some unit tests	3 months ago



ONTOLOGY STRUCTURE AND CONTENT

Ontology assembled from multiple sources



enonomapper (<http://purl.enonomapper.org/onto/enonomapper.owl>) : [C:\Work\Ontologies\enonomapper\ontologies\enonomapper.owl]

File Edit View Reasoner Tools Refactor Window Help

enonomapper (<http://purl.enonomapper.org/onto/enonomapper.owl>) Search for entity

Class matrix Annotation Properties Individuals Property matrix Individuals matrix OWLViz DL Query OntoGraf SPARQL Query

Active Ontology Entities Classes Object Properties Data Properties

Class hierarchy Class hierarchy (inferred) General class axioms

Class hierarchy: core

- ▶ 'environmental material'
- ▶ 'flat material part'
- ▶ 'chemical component'
- ▶ 'coat'
- ▶ core
 - ▶ 'dendrimer core'
 - ▶ 'inorganic core'
 - ▶ 'organic core'
 - ▶ 'dendrimer branch'
 - ▶ 'dendrimer generation layer'
 - ▶ 'flat dendrimer part'
 - ▶ 'linkage'
 - ▶ 'repeat unit'

Annotations: core

Annotations +

label [type: string]
core

code [type: string]
NPO_1617

definition [type: string]
`<ncicp:ComplexDefinition xmlns:ncicp="http://ncicb.nci.nih.gov/xml/owl/EVS/ComplexProperties.xsd#"><ncicp:def-definition>A flat material part which forms the basic structure or central part of an object</ncicp:def-definition><ncicp:Definition_Review_Date>100610</ncicp:Definition_Review_Date><ncicp:def-source>NPO</ncicp:def-source><ncicp:Definition_Reviewer_Name>Dennis Thomas</ncicp:Definition_Reviewer_Name><ncicp:ComplexDefinition>`

Individuals by type Annotation property hierarchy Datatypes

Object property hierarchy Data property hierarchy

Object property hierarchy:

- ▶ topObjectProperty

Description: core

Equivalent To +

SubClass Of +

▶ 'flat material part'

To use the reasoner click Reasoner->Start reasoner Show

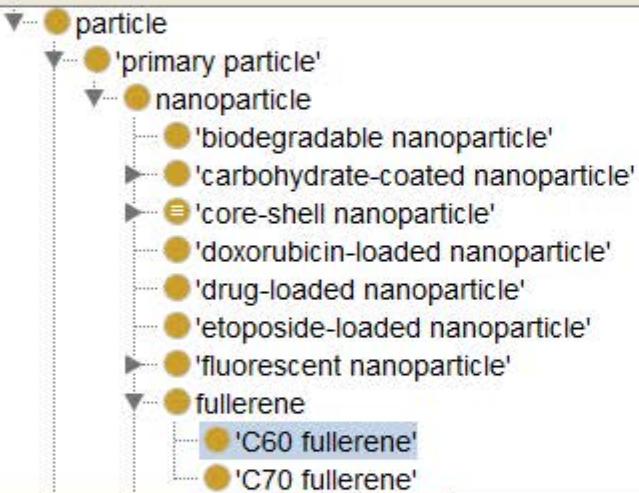


[enanomapper](#) (<http://purl.enanomapper.org/onto/enanomapper.owl>)

Annotation Properties Individuals Property matrix Individuals matrix OWLviz DL Query OntoGraf SPARQL Query
Active Ontology Entities Classes Object Properties Data Properties

Class hierarchy Class hierarchy (inferred) General class axioms

Class hierarchy: 'C60 fullerene'



Individuals by type Annotation property hierarchy Datatypes
Object property hierarchy Data property hierarchy

Object property hierarchy:



topObjectProperty

Selected entity Rules

Class Annotations Class Usage

Annotations: 'C60 fullerene'

Annotations

label [type: string]

C60 fullerene

Definition [type: string]

A fullerene that has formula C60.

InChI [type: string]

InChI=1S/C60/c1-2-5-6-3(1)8-12-10-4(1)9-11-7(2)17-21-13(5)23-24-14(6)22-18(8)28-20(12)30-26-16(10)15(9)25-29-19(11)27(17)37-41-31(21)33(23)43-44-34(24)32(22)42-38(28)48-40(30)46-36(26)35(25)45-39(29)47(37)55-49(41)51(43)57-52(44)50(42)56(48)59-54(46)53(45)58(55)60(57)59

InChIKey [type: string]

Description: 'C60 fullerene'

Equivalent To

SubClass Of

fullerene

To use the reasoner click Reasoner->Start reasoner

Show Inference

[enamomapper](#) (<http://purl.enanomapper.org/onto/enanomapper.owl>)

tox

Class matrix Annotation Properties Individuals Property matrix Individuals matrix OWLViz DL Query OntoGraf SPARQL Query
Active Ontology Entities Classes

Data Properties

Class hierarchy Class hierarchy (inferred) General class axioms

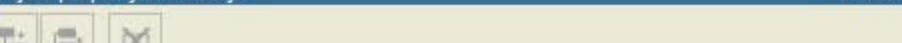
Class hierarchy: 'viral hemagglutination inhibition assay'

- 'activated partial thromboplastin time (aPTT) assay'
- 'age measurement assay'
- 'analyte assay'
- 'assay detecting IFN-gamma production'
- 'B cell epitope specific neutralization of antigen in vitro assay'
 - 'B cell epitope specific immunoglobulin-mediated neutralization assay'
 - 'viral hemagglutination inhibition assay'
- 'Bernoulli trial'
- 'binding assay'
- 'bioassay'
 - 'binding assay'
 - 'cell cycle assay'
 - 'cell growth assay'

Individuals by type Annotation property hierarchy Datatypes

Object property hierarchy Data property hierarchy

Object property hierarchy:



topObjectProperty

Selected entity Rules

Class Annotations Class Usage

Annotations: 'viral hemagglutination inhibition assay'

Annotations

label [type: string]

viral hemagglutination inhibition assay

'alternative term' [type: string]

HAI

'alternative term' [type: string]

viral hemeagglutination inhibition assay

definition [type: string]

a highly sensitive procedure for the measurement of soluble antigens in biologic specimens; the amount of hemagglutination reflects the amount of free antibody present after reaction with the specimen and thus varies inversely with amount of antigen in the specimen.

Description: 'viral hemagglutination inhibition assay'

Equivalent To

SubClass Of

'analyte assay'

To use the reasoner click Reasoner->Start reasoner

 Show Inference

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

size

Class matrix Annotation Properties Individuals Property matrix Individuals matrix OWLViz DL Query OntoGraf SPARQL Query
Active Ontology Entities Classes Object Properties Data Properties

Class hierarchy Class hierarchy (inferred) General class axioms

Class hierarchy: 'particle size distribution'



- intensity
- mass
- 'mass density'
- 'particle size'
- 'physical state'
- polydispersity
 - 'molecular weight distribution'
 - monodisperse
 - polydisperse
 - 'size distribution'
 - 'particle size distribution'
- porosity
- 'pour density'

Individuals by type Annotation property hierarchy Datatypes

Object property hierarchy Data property hierarchy

Object property hierarchy:

topObjectProperty

Selected entity Rules

Class Annotations Class Usage

Annotations: 'particle size distribution'

Annotations

- label [type: string]
particle size distribution
- code [type: string]
NPO_1699
- definition [type: string]

```
<ncicp:ComplexDefinition xmlns:ncicp="http://ncicb.nci.nih.gov/xml/owl/EVS/ComplexProperties.xsd#"><ncicp:def-definition>A size distribution inhering in particles.</ncicp:def-definition><ncicp:Definition_Review_Date>100430</ncicp:Definition_Review_Date><ncicp:Def-source>NPO</ncicp:Def-source><ncicp:Definition_Reviewer_Name>Dennis Thomas</ncicp:Definition_Reviewer_Name><ncicp:Definition_Reviewer_Name></ncicp:ComplexDefinition>
```

Description: 'particle size distribution'

Equivalent To

SubClass Of

- 'size distribution'

enanomapper (<http://purl.enanomapper.org/onto/enanomapper.owl>) : [C:\Work\Ontologies\enanomapper\ontologies\enanomapper.owl]

File Edit View Reasoner Tools Refactor Window Help

enanomapper (<http://purl.enanomapper.org/onto/enanomapper.owl>) Search for entity

Annotation Properties Class matrix Individuals Property matrix Individuals matrix OWLViz DL Query OntoGraf SPARQL Query Data Properties

Active Ontology Entities Classes Object Properties

Class hierarchy Class hierarchy (inferred)

Class hierarchy: carcinogenicity

Annotations Usage

Annotations: carcinogenicity

Annotations +

label [language: en]
carcinogenicity

definition
A toxicity disposition that inheres in a substance that is directly involved in causing cancer.

Description: carcinogenicity

Equivalent To +

SubClass Of +

toxicity

SubClass Of (Anonymous Ancestor)

Members +

Target for Key +

To use the reasoner click Reasoner->Start reasoner Show Inferences

The screenshot shows the enanomapper interface with the 'enanomapper' ontology loaded. On the left, the 'Class hierarchy' tab is selected, displaying a tree structure of classes under 'entity'. The 'carcinogenicity' class is highlighted in blue. The right panel shows the detailed view for the 'carcinogenicity' class, including its annotations (label and definition) and description properties (Equivalent To, SubClass Of, Members, Target for Key).

USING THE ONTOLOGY IN BIOPORTAL

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

eNanoMapper

Summary Classes Properties Notes Mappings Widgets

Details

ACRONYM	ENM
VISIBILITY	Public
BIOPORTAL PURL	http://purl.bioontology.org/ontology/ENM
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, egon.willighagen@gmail.com Janna Hastings, hastings@ebi.ac.uk
HOME PAGE	https://github.com/enanomapper/ontologies
PUBLICATIONS PAGE	
DOCUMENTATION PAGE	
CATEGORIES	Health
GROUPS	

Metrics

NUMBER OF CLASSES:	4555
NUMBER OF INDIVIDUALS:	177
NUMBER OF PROPERTIES:	652
MAXIMUM DEPTH:	10
MAXIMUM NUMBER OF CHILDREN:	91
AVERAGE NUMBER OF CHILDREN:	4
CLASSES WITH A SINGLE CHILD:	354
CLASSES WITH MORE THAN 25 CHILDREN:	34
CLASSES WITH NO DEFINITION:	1089

Visits

[Download as CSV](#)



Browse classes

eNanoMapper

Summary Classes Properties Notes Mappings Widgets

Jump To:

entity

- disposition
- information content entity
- material entity
- process
 - adverse event
 - assay
 - functionalization of nanoparticle
 - synthesis part
- quality

Details	Visualization	Notes (0)	Class Mappings ()	
Preferred Name	entity			
ID	http://purl.obolibrary.org/obo/BFO_0000001			
editor preferred label	entity			
label	entity			
prefixIRI	BFO:0000001			
prefLabel	entity			
subClassOf	http://www.w3.org/2002/07/owl#Thing			

View metadata (synonyms, ID)

eNanoMapper

Summary Classes Properties Notes Mappings Widgets

Jump To:

entity

- disposition
- information content entity
- material entity
- process
- quality
- concentration of dustiness
- hydrodynamic size
- intensity
- mass
- mass density
- particle size
- physical state
- polydispersity
- molecular weight distribution
- monodisperse
- polydisperse
- size distribution**

Details	Visualization	Notes (0)	Class Mappings (2)	🔗
Preferred Name	size distribution			
ID	http://purl.bioontology.org/ontology/npo#NPO_1697			
code	NPO_1697			
definition	A polydispersity inhering in a collection of objects based on size.			
FULL_SYN	size distributionPTNCI			
label	size distribution			
preferred_name	size distribution			
prefixIRI	npo:NPO_1697			
prefLabel	size distribution			
subClassOf	polydispersity			

Search

eNanoMapper

Summary Classes Properties Notes Mappings Widgets

Jump To:

entity

- + disposition
- + information content entity
- + material entity
- + process
 - + adverse event
 - + assay
 - + functionalization of nanoparticle
 - + synthesis part
- + quality

Details	Visualization	Notes (0)	Class Mappings ()	
Preferred Name	entity			
ID		http://purl.obolibrary.org/obo/BFO_0000001		
editor preferred label	entity			
label	entity			
prefixIRI	BFO:0000001			
prefLabel	entity			
subClassOf	http://www.w3.org/2002/07/owl#Thing			

Visualize

eNanoMapper

Summary Classes Properties Notes Mappings Widgets

Jump To:

Details

Visualization

Notes (0)

Class Mappings (2)

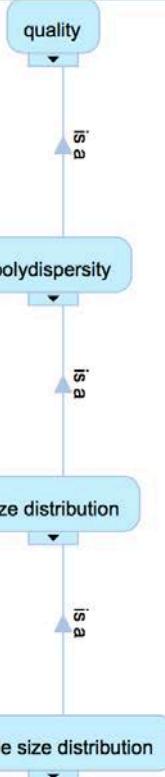
- entity
 - + disposition
 - + information content entity
 - + material entity
 - + process
 - quality
 - + concentration of dustiness
 - + hydrodynamic size
 - intensity
 - mass
 - + mass density
 - + particle size
 - + physical state
 - + polydispersity
 - molecular weight distribution
 - monodisperse
 - polydisperse
 - size distribution
 - particle size distribution
 - porosity
 - pour density
 - + rate
 - + shape
 - + solubility

Details

Visualization

Notes (0)

Class Mappings (2)



USING THE ONTOLOGY IN PROTEGE

Install Protégé:

<http://protege.stanford.edu>

- File → Open from URL: <http://purl.enanomapper.org/onto/enanomapper.owl>

The screenshot shows the Protégé ontology editor interface. At the top, there's a toolbar with standard browser-like buttons (back, forward, search) and tabs for Active Ontology, Entities, Classes, Object Properties, Data Properties, Annotation Properties, Individuals, OWLViz, DL Query, OntoGraf, SPARQL Query, and Ontology Differences. The Active Ontology tab is selected.

In the main area, there's a purple header bar labeled "Ontology header:" containing fields for "Ontology IRI" (set to <http://purl.enanomapper.org/onto/enanomapper.owl>) and "Ontology Version IRI" (set to e.g. <http://purl.enanomapper.org/onto/enanomapper.owl/1.0.0>). Below this, there's a section for "Annotations" with a plus sign icon. It lists several annotations:

- Contributor: Nina Jeliazkova (with edit and delete icons)
- comment: The eNanoMapper project (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.
- license: CC-BY 3.0 (<https://creativecommons.org/licenses/by/3.0/>) (with edit and delete icons)
- Contributor: Gareth Owen (with edit and delete icons)
- Contributor: Anna Hastings (with edit and delete icons)

Below the annotations, there's a purple header bar labeled "Ontology metrics:". Under "Metrics", there's a table with two rows:

Axiom	48483
Logical axiom count	5910

At the bottom, there are three tabs: "Ontology imports", "Ontology Prefixes", and "General class axioms".

Browse, Search

The screenshot shows the eNanoMapper ontology browser interface. At the top, there is a navigation bar with tabs: Active Ontology, Entities, Classes (highlighted with a red circle), Object Properties, Data Properties, Annotation Properties, Individuals, OWLviz, DL Query, OntoCraf, SPARQL Query, and Ontology Difference.

The main area has two main sections:

- Class hierarchy:** 'epigenetic modification assay' (highlighted with a red circle). This section displays a tree view of the ontology classes. The root node 'entity' has several children, including 'disposition', 'information content entity', 'material entity', 'process', and 'assay'. The 'assay' node has many sub-classes listed, such as 'adverse event', 'activated partial thromboplastin time', 'age measurement assay', 'analyte assay', 'array based nucleic acid structure', 'assay detecting IFN-gamma production', 'assay for transposase-accessible chromatin', 'B cell epitope specific neutralization', 'Bernoulli trial', 'binding assay', 'bioassay', 'cell mediated cell killing assay', 'cell proliferation assay', 'comet assay', 'copy number variation profiling', 'cytochalasin-induced inhibition assay', 'detection of molecular label', 'DNA replication timing by array assay', 'DNA sequence feature detection', 'DNA sequence variation detection', 'efficacy of epitope intervention experiment', 'ELISPOT assay', 'epigenetic modification assay' (which is highlighted with a blue box), and 'extracellular electrophysiology recording'.
- Annotations:** 'epigenetic modification assay' (highlighted with a red circle). This section shows various annotations for the entity. It includes:
 - label:** epigenetic modification assay
 - definition:** An assay that identifies epigenetic modification including histone modifications, open chromatin, and DNA methylation.
 - 'definition source':** Penn group
 - 'editor preferred term':** epigenetic modification assay
 - 'has curation status':** **'metadata complete'** (marked with a diamond icon)
 - Source:** Beta Cell Biology Consortium

Logic-based querying

DL query:

Query (class expression)

```
bioassay and 'has endpoint' some 'concentration endpoint'
```

Execute

Add to ontology

Query results

Sub classes (2)

● 'KiNativ assay'

REQUESTING CHANGES

GitHub enanomapper ontologies

enannomapper / ontologies

Watch 15 Star 0 Fork 1

Issues Pull requests Labels Milestones Filters is:issue is:open New issue

21 Open 4 Closed

Author Labels Milestones Assignee Sort

Incorporation of several URIs from new and already used ontology resources #25 opened 6 days ago by Irieswijk

endpoints to be added #24 opened 28 days ago by vedina

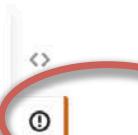
NM_001005 describes both particle size and zeta potential ENM #23 opened 28 days ago by vedina

protocol and assay type entries #22 opened 29 days ago by vedina

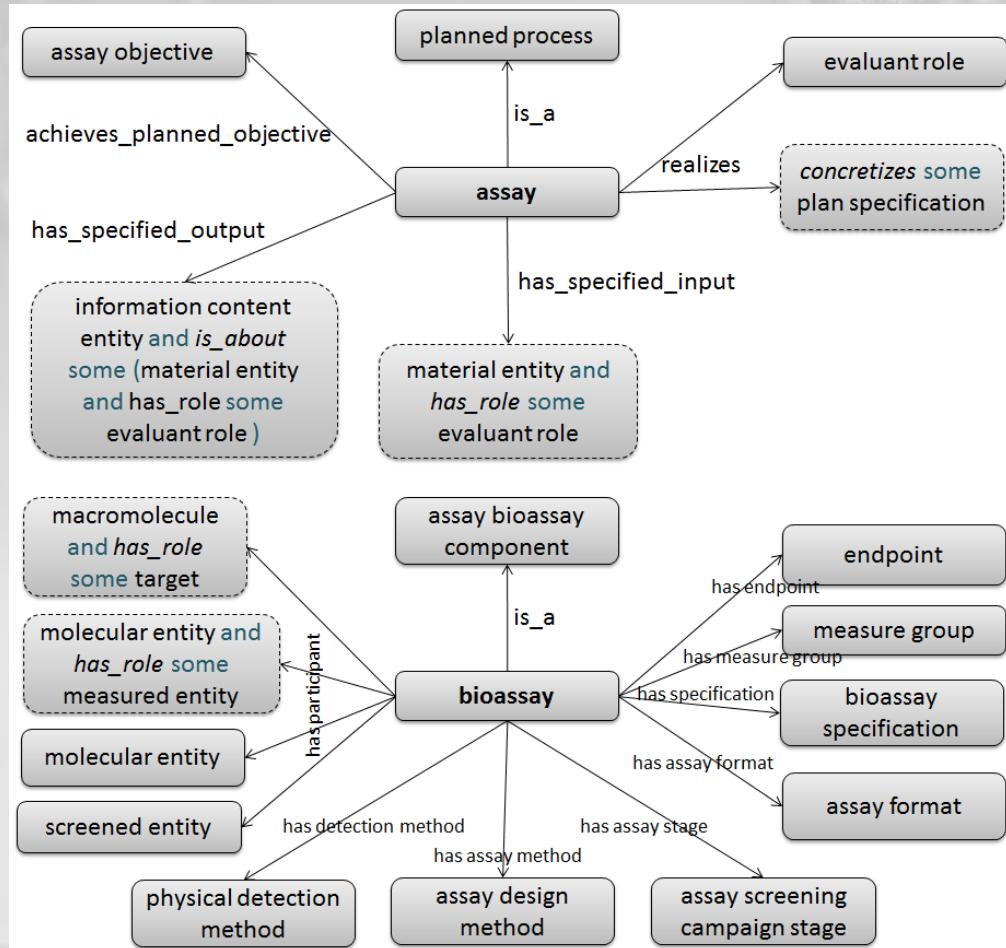
Add National Cancer Institute Thesaurus to ontology #21 opened 29 days ago by Irieswijk

Merge 'toxicity' and 'toxicity endpoint' branches #20 opened on May 13 by jannahastings

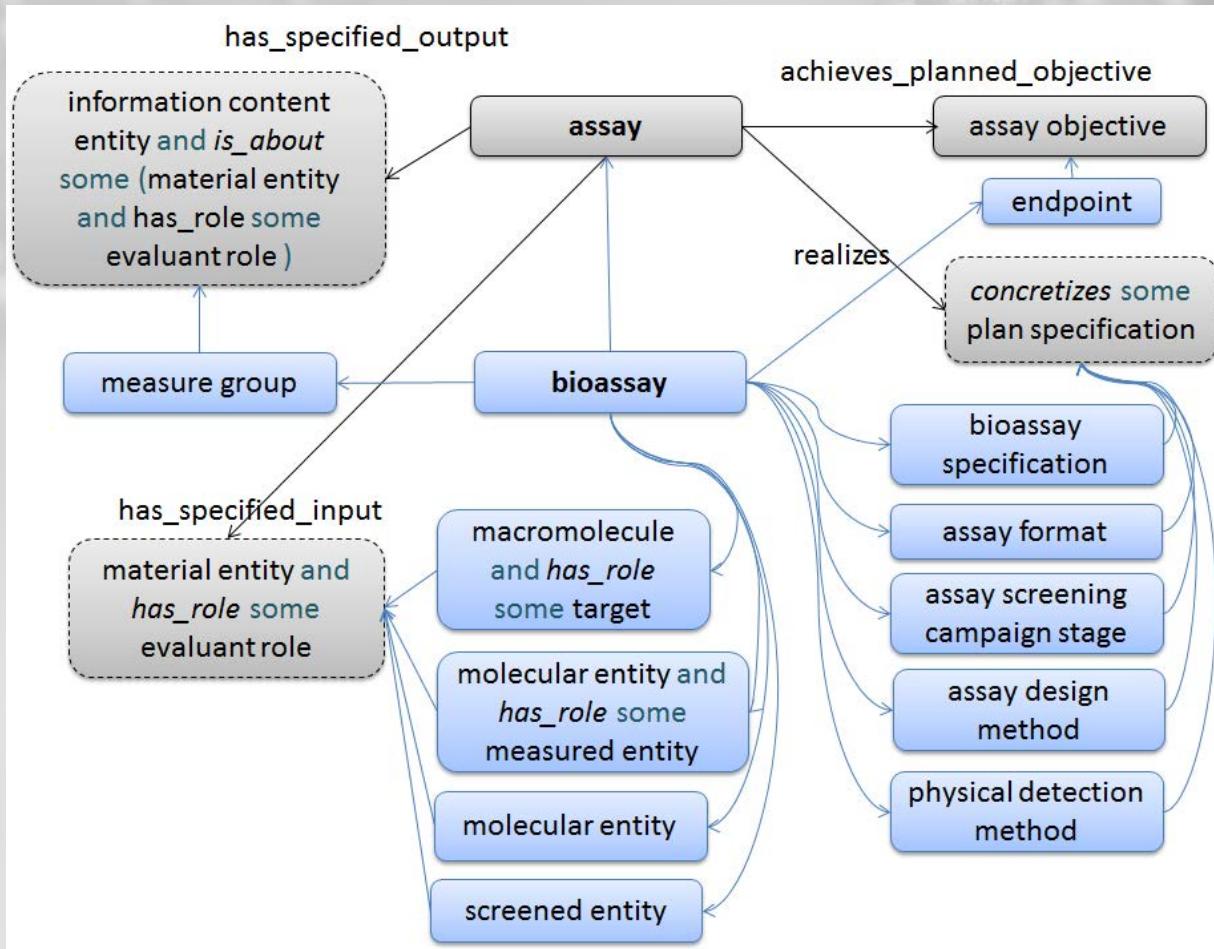
include STATO for e.g. min/max #19 opened on May 12 by jannahastings



Relationship/model harmonization



Relationship/model harmonization



Acknowledgements

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grant agreement no 604134 within the
7th Framework Programme for research
and technological development.



Questions?