Using the eNanoMapper ontology

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EMBL-EBI

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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

<table>
<thead>
<tr>
<th>File</th>
<th>Description</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>src</td>
<td>Update npo.iris</td>
<td>6 days ago</td>
</tr>
<tr>
<td>.gitignore</td>
<td>It can now read an ontology</td>
<td>4 months ago</td>
</tr>
<tr>
<td>.project</td>
<td>Found the culprit</td>
<td>4 months ago</td>
</tr>
<tr>
<td>LICENSE</td>
<td>Create LICENSE</td>
<td>2 months ago</td>
</tr>
<tr>
<td>README.md</td>
<td>Added more detail about how Slimmer works</td>
<td>9 days ago</td>
</tr>
<tr>
<td>pom.xml</td>
<td>Added some unit tests</td>
<td>3 months ago</td>
</tr>
</tbody>
</table>
1. Configuration file
   - Initialise, read instructions
   - Parse input OWL file, flatten imports
   - Remove content not specifically included in instructions
   - Remove content specifically excluded in instructions
   - Generate output file

2. Slimming instruction file
   - Input OWL file
   - Imported OWL dependency files
   - Output OWL file
ONTOGONY STRUCTURE AND CONTENT
Ontology assembled from multiple sources

- Disposition
- Material entity
- Process
- Quality

- Bioavailability
- Toxicity
- Environmental toxicity
- Carcinogenicity
- Oral toxicity

- Information content entity
- Chemical descriptor
- Endpoint
- Bioassay
- Unit
- Chemical entity
- Chemical substance
- Nanomaterial
- Nanoparticle

- Synthesis part
- Hydrodynamic size
- Polydispersity
- Pour density
- Concentration

- 4,456 classes
A fullerene that has formula C60.

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)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 = 8echMv9L58H8AR

topObjectProperty

equivalentTo

SubClassOf fullerene
'viral hemagglutination inhibition assay' is 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.
Class hierarchy: 'particle size distribution'

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

Object property hierarchy:

- topObjectProperty

Representations:

**Annotatios:**
- **label**: string
  - particle size distribution
- **code**: string
  - NPO_1699

**Definition**:

```xml
```
Annotations: carcinogenicity

- label [language: en]
  - carcinogenicity

Definition:
A toxicity disposition that inheres in a substance that is directly involved in causing cancer.
USING THE ONTOLOGY IN BIOPORTAL
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.

**Details**

<table>
<thead>
<tr>
<th>Field</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td><strong>ACRONYM</strong></td>
<td>ENM</td>
</tr>
<tr>
<td><strong>VISIBILITY</strong></td>
<td>Public</td>
</tr>
<tr>
<td><strong>BIOPORTAL PURL</strong></td>
<td><a href="http://purl.bioontology.org/ontology/ENM">http://purl.bioontology.org/ontology/ENM</a></td>
</tr>
<tr>
<td><strong>DESCRIPTION</strong></td>
<td>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.</td>
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<td><strong>STATUS</strong></td>
<td>Alpha</td>
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<tr>
<td><strong>FORMAT</strong></td>
<td>OWL</td>
</tr>
<tr>
<td><strong>CONTACT</strong></td>
<td>Egon Willighagen, <a href="mailto:egon.willighagen@gmail.com">egon.willighagen@gmail.com</a> Janna Hastings, <a href="mailto:hastings@ebi.ac.uk">hastings@ebi.ac.uk</a></td>
</tr>
<tr>
<td><strong>HOME PAGE</strong></td>
<td><a href="https://github.com/enanomapper/ontologies">https://github.com/enanomapper/ontologies</a></td>
</tr>
<tr>
<td><strong>PUBLICATIONS PAGE</strong></td>
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<td><strong>DOCUMENTATION PAGE</strong></td>
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<td><strong>CATEGORIES</strong></td>
<td>Health</td>
</tr>
<tr>
<td><strong>GROUPS</strong></td>
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</tr>
</tbody>
</table>

**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

#### Classes

<table>
<thead>
<tr>
<th>Jump To:</th>
<th>Details</th>
<th>Visualization</th>
<th>Notes (0)</th>
<th>Class Mappings (0)</th>
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<tbody>
<tr>
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<td>Preferred Name</td>
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<tr>
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<td>entity</td>
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<td>prefixIRI</td>
<td>BFO:0000001</td>
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<td>entity</td>
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<tr>
<td></td>
<td>subClassOf</td>
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<td></td>
<td></td>
</tr>
</tbody>
</table>
### View metadata (synonyms, ID)

**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

**prefixLabel:** size distribution

**subClassOf:** polydispersity
Visualize
USING THE ONTOLOGY IN PROTEGE
Install Protégé:
http://protege.stanford.edu

- File ➔ Open from URL: http://purl.enanomapper.org/onto/enanomapper.owl
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
Relationship/model harmonization
Relationship/model harmonization
eNanoMapper is funded by the EU, grant agreement no 604134 within the 7th Framework Programme for research and technological development.
Questions?