

Expanding the eNanoMapper Ontology

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Introduction

Matching the developmental rate of novel NMs with research and safety regulations is a **challenging task**. To accelerate the transition to *in silico* nanosafety, the NanoSafety Cluster identified the need for an infrastructure for toxicological data management and nanoinformatics.

The **NanoCommons** Knowledgebase, <https://www.nanocommons.eu/nanocommons-knowledge-base/>, is an essential component of nanoinformatics and based on an agreed ontology. NanoCommons has continued to expand and develop the **eNanoMapper (ENM)** ontology to aid toxicological data management for NMs [1]. Ontological mapping facilitates the organization, integration and reuse of data which suits the premise of less usage of animals for research purposes.

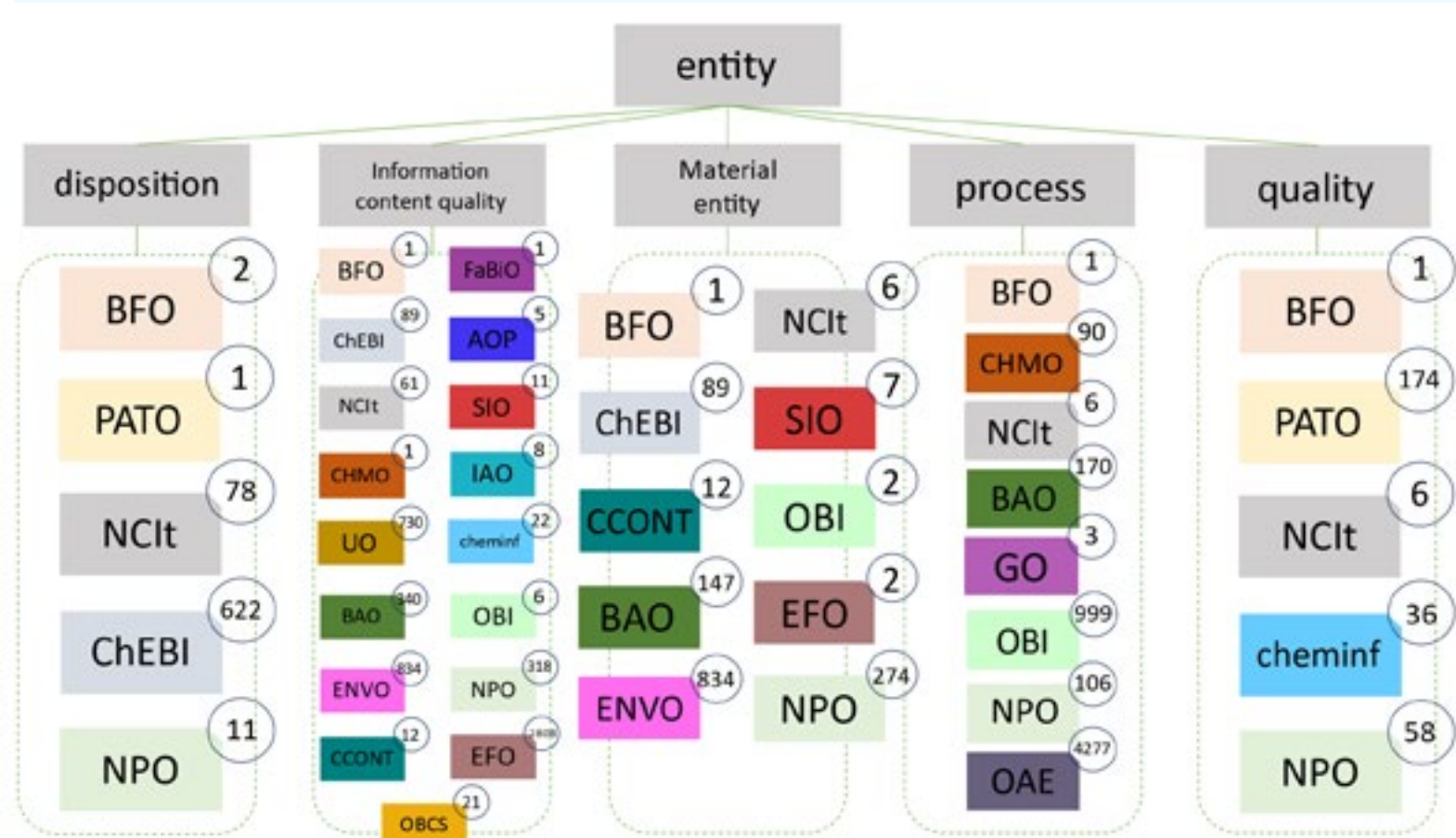


Figure 1. Distribution of number of classes per ontology as subclass of five parent classes which have the shared parent class; *entity*.

Methods

The latest release of the **eNanoMapper ontology (ENM)**, version 6.0, was acquired via Zenodo, <https://doi.org/10.5281/zenodo.3382100>. **ROBOT is an OBO Tool (ROBOT)** was used as a command-line tool to work with the ENM ontology. ROBOT was set up according to their instructions and was used in Windows Command Prompt [2]. The **OBO Dashboard**, acquired from <https://github.com/OBOFoundry/OBO-Dashboard>, was used to assess the quality and validate the ENM ontology [3].

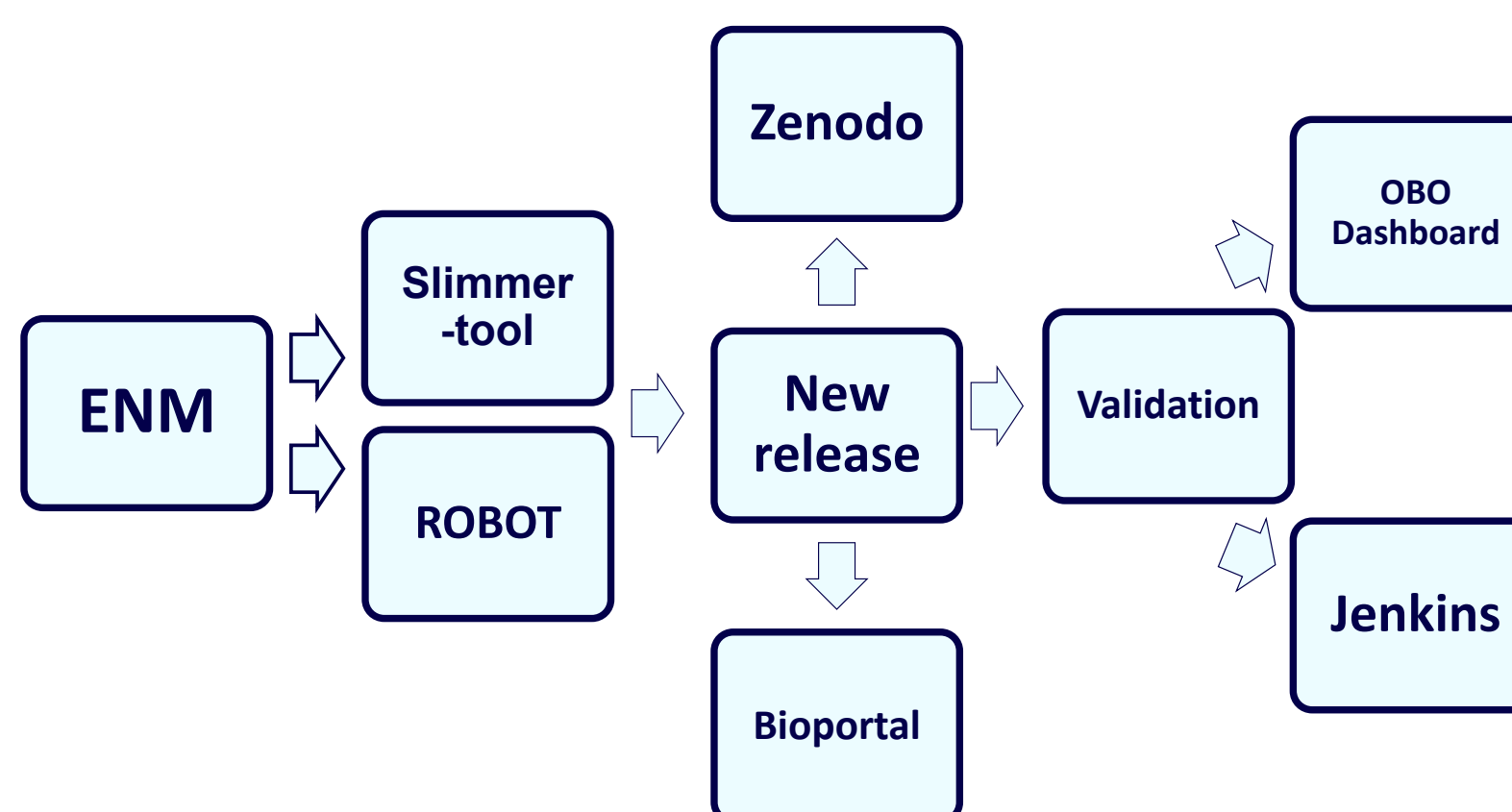


Figure 2. Workflow for extension, development and maintenance of the eNanoMapper (ENM) ontology. First the previous version of the ENM ontology will be extended with terms and properties which were extracted using ROBOT and slimmed versions of initial ontologies. These will be merged with the ENM ontology to create a new release on Zenodo and Bioportal, which subsequently, will be validated using OBO Dashboard and Jenkins.

```

> sh ./robot filter --input npo-inferred.owl \
> --branch-from-term "http://purl.bioontology.org/ontology/npo#has_part" \
> --select annotations --output npo-slim.owl
  
```

Figure 3. ROBOT's filter command. Extracting annotation property *has_part* from the Nanoparticle Ontology (NPO) [4].

```

> wget \
https://raw.githubusercontent.com/enanmapper/ontologies/master/config/SIO-term-file.txt
> sh ./robot filter --input sio.owl --term-file sio-term-file.txt --select \
> annotations --output SIO-slim.owl
  
```

Figure 4. ROBOT's filter command. Extracting multiple annotation properties stored in a list from the Semanticscience Integrated Ontology (SIO) [5].

Results

We were able to recreate the eNanoMapper ontology using **ROBOT's MERGE command**. We were able to extract annotation properties from the Nanoparticle Ontology, Chemical Information Ontology, Semanticscience Integrated Ontology and BioAssay Ontology which were previously identified as being absent from the ENM ontology, with the **ROBOT's FILTER command**. We were able to import these annotation properties into the ENM ontology.

In addition, we were not able yet to use the OBO Dashboard to assess and validate the ENM ontology, as the ENM ontology is not registered at the OBO foundry. A workaround could be to manually assess the ENM ontology based on the same test the OBO Dashboard uses.

Conclusion

A major improvement to the ENM ontology development is the extension with annotation properties. **ROBOT** was found to be an **easy-to-use** and **suitable** tool to achieve this. In addition, the **OBO Dashboard** will be **useful** to assess and validate the ENM ontology, which provides an improved workflow in which we will **continue to develop and maintain** the eNanoMapper ontology as part of the NanoCommons research infrastructure for nanosafety data management and nanoinformatics.

References

- Hastings J, Jeliaskova N, Owen G, Tsiliki G, Munteanu CR, Steinbeck C, Willighagen EL. eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment. *J Biomed Semantics*. 2015;6:10. doi: 10.1186/s13326-015-0005-5
- Jackson, RC, Balhoff, JP, Douglass, E. *et al*. ROBOT: A Tool for Automating Ontology Workflows. *BMC Bioinformatics*. 2019;20:407. doi: 10.1186/s12859-019-3002-3
- Smith B, *et al*. The OBO Foundry: coordinated evolution of ontologies to support biomedical data integration. *Nat Biotech* 2007;25 doi: 10.1038/nbt1346.
- Thomas DG, Pappu RV, Baker NA. Nanoparticle Ontology for Cancer Nanotechnology Research. *J Biomed Inform*. 2011;44:1. doi: 10.1016/j.jbi.2010.03.0014.
- Dumontier M, *et al*. The Semanticscience Integrated Ontology (SIO) for biomedical research and knowledge discovery. *J Biomed Semantics* 2014;6:5(1). doi: 10.1186/2041-1480-5-14.