Expanding the eNanoMapper Ontology

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Keywords. eNanoMapper, NanoCommons, EU NanoSafety Cluster, ontology, nanomaterial, engineered nanomaterial, nanoinformatics

1. Introduction

The NanoSafety Cluster (NSC) is a cluster of projects funded by the European Commission to assess the environmental health and safety of engineered nanomaterials (NMs). Many (new) NMs are being developed for specific applications within multiple fields such as healthcare/biomedical sciences and the industry. They are categorized depending on their size, composition, shape and origin.

Matching the developmental rate of novel NMs with research and safety regulations is a challenging task. Additionally, regulators have decided that the number of animals used in research should be as low as possible. Whereas cytotoxicity testing from *in vitro* to *in vivo* would take up too much time and resources, such as animals and money, to keep up with the increasing prominence of NMs, the development and validation of *in silico* toxicology and nanoinformatics are still at an early stage. To accelerate the transition to *in silico* nanosafety, the NSC identified the need for an infrastructure for toxicological data management and nanoinformatics, NanoCommons, https://www.nanocommons.eu/nanocommons-knowedge-base/. An essential component of nanoinformatics is an agreed ontology, and NanoCommons has continued to expand and develop the eNanoMapper (ENM) ontology to aid toxicological data management for NMs [1]. Ontological mapping facilitates the organisation, integration and reuse of data which suits the premise of less usage of animals for research purposes.

Besides continuous collaboration with the NSC on the identification of missing terms and additional existing ontologies to build upon, within NanoCommons we have examined an approach to extend the current ontology with new properties. We used the recently published *ROBOT is an OBO Tool* [2] to extend the ENM ontology with missing annotation properties from, for example, the NanoParticle Ontology [3]. In addition, we have used the OBO Dashboard to assess the quality and validate the ENM ontology to assess the level of compliance with OBO Principles and best practises [3,4].

2. Methods

The latest release of the eNanoMapper ontology (ENM), version 4.0, was acquired via

Zenodo, https://doi.org/10.5381/zenodo.260098.
The NanoParticle Ontology (NPO), https://bioportal.bioontology.org/ontologies/NPO, was used to extract annotation properties which were not found in the ENM ontology.
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.
The OBO Dashboard, acquired from https://github.com/OBOFoundry/OBO-Dashboard, was used to assess the quality and validate the ENM ontology.

3. Preliminary results

The ENM ontology could not directly be used in ROBOT as the OWL file uses *owl:imports* of slimmed ontologies. This led to the recreation of the ENM ontology using the MERGE command. The slimmed ontologies were merged and resulted in the recreation of the eNanoMapper ontology as found on https://www.nanocommons.eu/. Upon recreation of the ENM ontology, the resulting OWL file could be used for other ROBOT commands. Additionally, we were able to extract annotation properties from the NanoParticle Ontology such as *npo:has_part*, which were previously identified as being absent from the ENM ontology, with the ROBOT's EXTRACT command. We were able to import these annotation properties into the ENM ontology. In addition, we were able to use the OBO Dashboard to assess and validate the ENM ontology. The OBO Dashboard prompted a report which assessed multiple aspects of the ontology and provided errors if applicable. For example, *missing ontology license* and *missing definitions* are common error messages.

4. 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 was 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

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