



Ontology, database and tools for nanomaterial safety evaluation

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Introduction

Nanomaterials are defined by size: between 1 and 100 nm in at least one dimension. The properties of these material do not always resemble those of the bulk material, i.e. micro- and bigger particles, or solutions. Nanomaterials differ in reactivity, toxicity in biological organisms and ecosystems depending on their size and surface properties and the possibility for "leakage" of the material it is made off. It is difficult to assess the safety of nanomaterials and therefore the NanoSafety Cluster defined a need for a new computational infrastructure in 2012. eNanoMapper is a European project with partners from eight European countries. This project developed www.enanomapper.net a semantic web assisted database, a modular ontology, and tools to use them for nanomaterial safety assessment. Data sharing, data storage, data analysis tools, and web services are currently being developed, tested, and put into production use.

Problem

The eNanoMapper platform supports hosting of data on nanomaterial properties relevant for nanosafety assessment as found in existing databases like the NanoMaterial Registry, DaNa Knowledge Base, Nanoparticle Information Library NIL, Nanomaterial-Biological Interactions Knowledgebase, caNanoLab, InterNano, Nano-EHS Database Analysis Tool, nanoHUB, etc. Each has different data formats and descriptors, like CODATA-VAMAS' Universal Description System, ISO-Tab(-Nano), OECD templates, custom spreadsheets, and images. Interoperability is a main aim and semi-automatic import or upload of information and to integrate it in the eNanoMapper data structure is being enabled. *Vice versa*, retrieval or download of experimental data from the database for (re-)analysis should be provided too, using programmable interfaces to the data and the ontology.

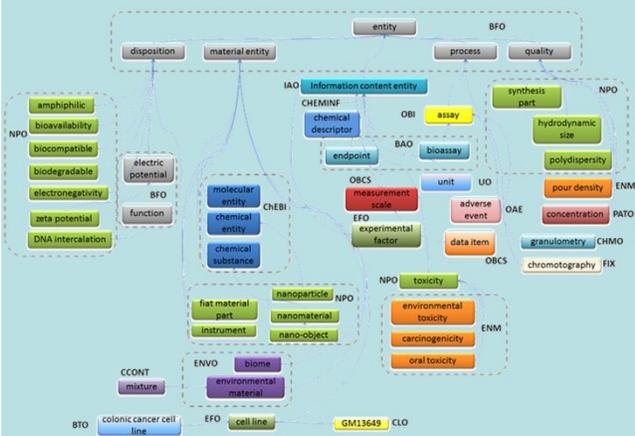


Figure 1: An overview of the upper levels and integration of external ontology content (18 ontologies) together with manually annotated (ENM) content (comprises >6690 classes)

Database and search functionality should be semantic web compatible: the project developed and maintain a nanosafety ontology to support this. This eNanoMapper ontology was developed using the Web Ontology Language (OWL) and the challenge is to map nanomaterial terms to their multiple ontology terms, namely physico-chemical properties, biological and ecological impact, experimental assay description, and known safety aspects (Figure 1).

References

- Jeliaskova, N. et al. The eNanoMapper database for nanomaterial safety information. *Beilstein Journal of Nanotechnology* 6, 1609-1634, doi:10.3762/bjnano.6.165 (2015).
- Willighagen, E.; doi: org/10.6084/m9.figshare.1330208 (2015).
- Hastings, J. et al. eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment. *J Biomed Semantics* 6, 10, doi:10.1186/s13326-015-0005-5 (2015).

Results and Discussion

The current eNanoMapper demo database instance, available at data.enanomapper.net/, contains the physico-chemical, biologic and environmental properties of nanomaterials of 465 different nanomaterials¹. Loading data into the database supports various formats, including the OECD Harmonized Templates and the data structure used by the NanoWiki². A web interface is designed to support all interactions with the database you may want to perform, including uploading of experimental data, as well as querying data to support analysis and modelling of nanoparticle properties (Figure 2).

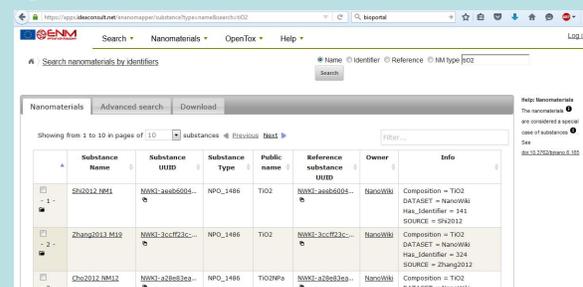


Figure 2: The eNanoMapper database, a repository of nanomaterial safety data and information.

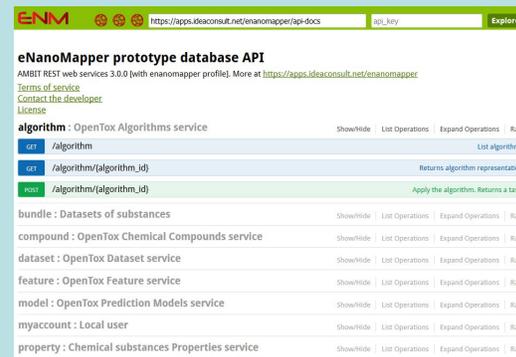


Figure 3: List of some current eNanoMapper APIs, more at apps.ideaconsult.net/enanomapper

The eNanoMapper ontology is available under purl.enanomapper.net/onto/enanomapper.owl and is based on a multi-faceted description of nanoparticles concerning nanoparticle types, physico-chemical description, life cycle, biological and environmental characterisation including experimental methods and protocols, and safety information³. The terms are verified against the definitions of REACH, ISO, or common practices used in science in general. The often confused different meanings of endpoints and assays were discriminated in the definitions, e.g. size and size measurement assay. It was partly possible to use existing ontologies as basis, e.g. NPO, ChEBI, GO, etc. but many terms had to be added manually. Currently, there are 4592 classes defined. Users can get access and download the ontology from the U.S. National Center for BioMedical Ontologies BioPortal platform, or AberOWL.

Associate Partner Program

www.enanomapper.net/associate-partner-program

The associate partner program facilitates collaborations between outside organizations and eNanoMapper towards the common goals of the nanosafety community. Collaboration is communicated by including all partners on the eNanoMapper website, as well as eNanoMapper on the partners' web sites. Other obligations, such as involving confidentiality, work commitments or shared intellectual properties are explicitly not part of the program and are the subject of other agreements such as inter-consortium agreements.



Douglas Connect
Working collaboratively



in silico toxicology



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