

# FAIR for NanoSafety: where do we stand?

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NanoWG

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# Why FAIR?

Reusable.



# Why FAIR?

Reusable.

But how do we make something (theoretically) reusable?

- findable
- accessible
- interoperable



# Findable, Accessible, Interoperable, Reusable



F1: identifiers, F2: rich metadata, F3: registered or indexed, F4: specify identifiers

A1: standard protocols, A2: metadata persistent

I1: common language, I2: FAIR vocabularies, I3: references other FAIR

R1: clear license, provenance, community standards

SCIENTIFIC DATA

[Comment](#) | [OPEN](#) | [Published: 15 March 2016](#)

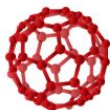
The FAIR Guiding Principles for scientific data management and stewardship

[Mark D. Wilkinson](#), [Michel Dumontier](#) [...] [Barend Mons](#)

*Scientific Data* **3**, Article number: 160018 (2016) | [Download Citation](#)



# F1: persistent identifiers



## eNanoMapper Ontology IRIs for the OECD nanomaterials

eNanoMapper Working Draft 18 October 2017

**This version:**

<http://specs.enanomapper.org/2017/WD-oecd-20171018/>

**Latest published version:**

<http://specs.enanomapper.org/oecd/>

**Previous version:**

none

**Editor:**

[Egon Willighagen](#), [Maastricht University](#)

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### Abstract

OECD nanomaterial	Code	Full Ontology IRI
cerium oxide nanoparticles	ENM_9000006	<a href="http://purl.enanomapper.org/onto/ENM_9000006">http://purl.enanomapper.org/onto/ENM_9000006</a>
multi-walled carbon nanotubes	NPO_354	<a href="http://purl.bioontology.org/ontology/npo#NPO_354">http://purl.bioontology.org/ontology/npo#NPO_354</a>
single-walled carbon nanotubes	NPO_943	<a href="http://purl.bioontology.org/ontology/npo#NPO_943">http://purl.bioontology.org/ontology/npo#NPO_943</a>
dendrimers	NPO_735	<a href="http://purl.bioontology.org/ontology/npo#NPO_735">http://purl.bioontology.org/ontology/npo#NPO_735</a>
nanoclay nanoparticles	ENM_9000007	<a href="http://purl.enanomapper.org/onto/ENM_9000007">http://purl.enanomapper.org/onto/ENM_9000007</a>
titanium dioxide nanoparticles	CHEBI_51050	<a href="http://purl.obolibrary.org/obo/CHEBI_51050">http://purl.obolibrary.org/obo/CHEBI_51050</a>
fullerenes	CHEBI_33128	<a href="http://purl.obolibrary.org/obo/CHEBI_33128">http://purl.obolibrary.org/obo/CHEBI_33128</a>
silicon dioxide nanoparticles	NPO_1373	<a href="http://purl.bioontology.org/ontology/npo#NPO_1373">http://purl.bioontology.org/ontology/npo#NPO_1373</a>
zinc oxide nanoparticles	NPO_1542	<a href="http://purl.bioontology.org/ontology/npo#NPO_1542">http://purl.bioontology.org/ontology/npo#NPO_1542</a>
gold nanoparticles	NPO_401	<a href="http://purl.bioontology.org/ontology/npo#NPO_401">http://purl.bioontology.org/ontology/npo#NPO_401</a>
silver nanoparticles	NPO_1892	<a href="http://purl.bioontology.org/ontology/npo#NPO_1892">http://purl.bioontology.org/ontology/npo#NPO_1892</a>
iron nanoparticles	ENM_9000200	<a href="http://purl.enanomapper.org/onto/ENM_9000200">http://purl.enanomapper.org/onto/ENM_9000200</a>
aluminium oxide nanoparticles	ENM_9000005	<a href="http://purl.enanomapper.org/onto/ENM_9000005">http://purl.enanomapper.org/onto/ENM_9000005</a>



# F1: persistent identifiers



## eNanoMapper Ontology IRIs for the JRC representative industrial nanomaterials

eNanoMapper Working Draft 20 January 2018

### This version:

<http://specs.enanomapper.org/2018/WD-jrc-20180120/>

### Latest published version:

<http://specs.enanomapper.org/jrc/>

### Previous version:

<http://specs.enanomapper.org/2017/WD-jrc-20170226/>

### Editor:

[Egon Willighagen](#), [Maastricht University](#)

### Author:

Jiakang Chang, [EMBL-FBI](#)

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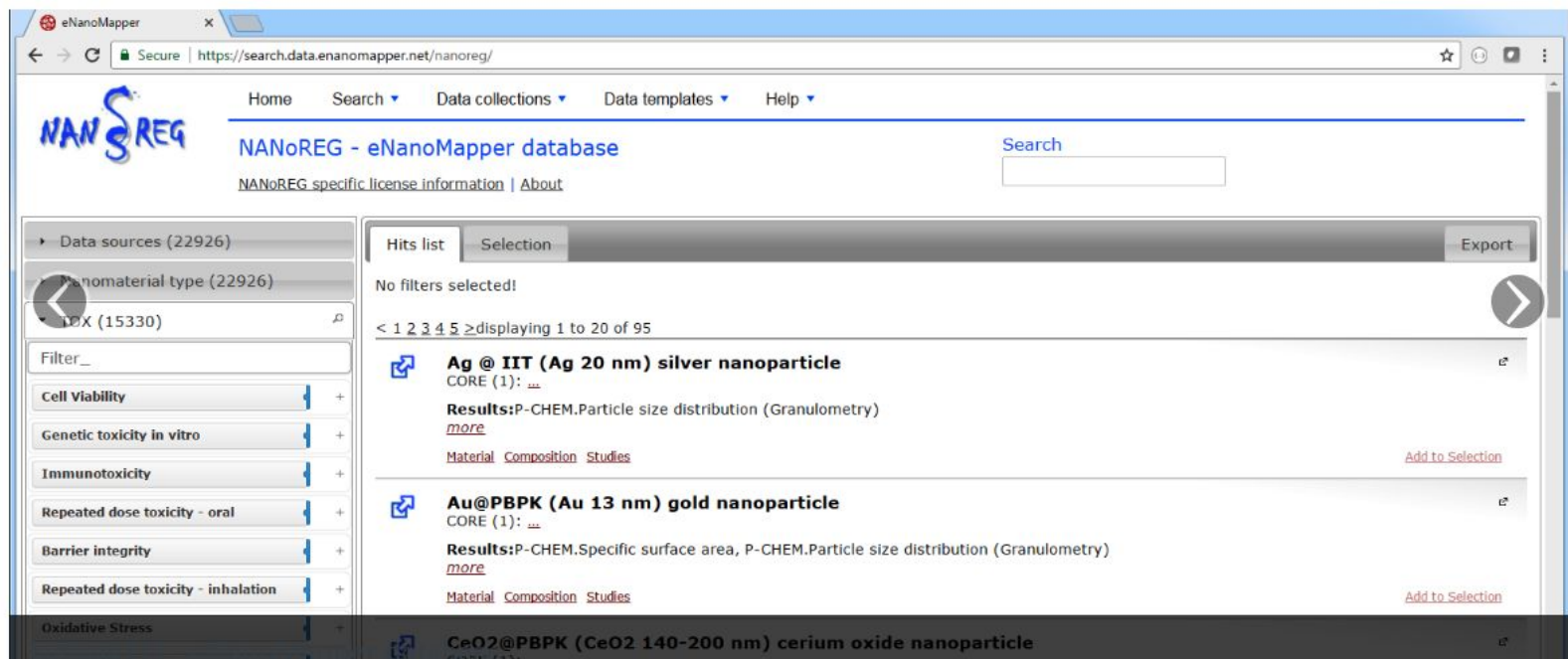
## Abstract

JRC nanomaterial Code	Ontology IRI	Wikidata
JRCNM01000a	ENM_9000074 <a href="http://purl.enanomapper.org/onto/ENM_9000074">http://purl.enanomapper.org/onto/ENM_9000074</a>	<a href="#">Q27918612</a>
JRCNM01001a	ENM_9000075 <a href="http://purl.enanomapper.org/onto/ENM_9000075">http://purl.enanomapper.org/onto/ENM_9000075</a>	<a href="#">Q47461406</a>
JRCNM01002a	ENM_9000076 <a href="http://purl.enanomapper.org/onto/ENM_9000076">http://purl.enanomapper.org/onto/ENM_9000076</a>	<a href="#">Q47461416</a>
JRCNM01003a	ENM_9000083 <a href="http://purl.enanomapper.org/onto/ENM_9000083">http://purl.enanomapper.org/onto/ENM_9000083</a>	<a href="#">Q47461418</a>
JRCNM01004a	ENM_9000084 <a href="http://purl.enanomapper.org/onto/ENM_9000084">http://purl.enanomapper.org/onto/ENM_9000084</a>	<a href="#">Q47461419</a>
JRCNM01005a	ENM_9000077 <a href="http://purl.enanomapper.org/onto/ENM_9000077">http://purl.enanomapper.org/onto/ENM_9000077</a>	<a href="#">Q47461422</a>
JRCNM01100a	ENM_9000078 <a href="http://purl.enanomapper.org/onto/ENM_9000078">http://purl.enanomapper.org/onto/ENM_9000078</a>	<a href="#">Q47462004</a>
JRCNM01101a	ENM_9000086 <a href="http://purl.enanomapper.org/onto/ENM_9000086">http://purl.enanomapper.org/onto/ENM_9000086</a>	<a href="#">Q47462008</a>
JRCNM02000a	ENM_9000087 <a href="http://purl.enanomapper.org/onto/ENM_9000087">http://purl.enanomapper.org/onto/ENM_9000087</a>	<a href="#">Q47462022</a>
JRCNM02001a	ENM_9000088 <a href="http://purl.enanomapper.org/onto/ENM_9000088">http://purl.enanomapper.org/onto/ENM_9000088</a>	<a href="#">Q47468470</a>
JRCNM02002a	ENM_9000089 <a href="http://purl.enanomapper.org/onto/ENM_9000089">http://purl.enanomapper.org/onto/ENM_9000089</a>	<a href="#">Q47468473</a>
JRCNM02003a	ENM_9000090 <a href="http://purl.enanomapper.org/onto/ENM_9000090">http://purl.enanomapper.org/onto/ENM_9000090</a>	
JRCNM02004a	ENM_9000091 <a href="http://purl.enanomapper.org/onto/ENM_9000091">http://purl.enanomapper.org/onto/ENM_9000091</a>	<a href="#">Q47468478</a>
JRCNM02004b	ENM_9000092 <a href="http://purl.enanomapper.org/onto/ENM_9000092">http://purl.enanomapper.org/onto/ENM_9000092</a>	
JRCNM02101a	ENM_9000237 <a href="http://purl.enanomapper.org/onto/ENM_9000237">http://purl.enanomapper.org/onto/ENM_9000237</a>	
JRCNM02102a	ENM_9000238 <a href="http://purl.enanomapper.org/onto/ENM_9000238">http://purl.enanomapper.org/onto/ENM_9000238</a>	<a href="#">Q47461933</a>
JRCNM03300a	ENM_9000097 <a href="http://purl.enanomapper.org/onto/ENM_9000097">http://purl.enanomapper.org/onto/ENM_9000097</a>	
JRCNM03301a	ENM_9000098 <a href="http://purl.enanomapper.org/onto/ENM_9000098">http://purl.enanomapper.org/onto/ENM_9000098</a>	
JRCNM04000a	ENM_9000080 <a href="http://purl.enanomapper.org/onto/ENM_9000080">http://purl.enanomapper.org/onto/ENM_9000080</a>	<a href="#">Q47462019</a>
JRCNM04001a	ENM_9000081 <a href="http://purl.enanomapper.org/onto/ENM_9000081">http://purl.enanomapper.org/onto/ENM_9000081</a>	<a href="#">Q47462603</a>
JRCNM10201a	ENM_9000094 <a href="http://purl.enanomapper.org/onto/ENM_9000094">http://purl.enanomapper.org/onto/ENM_9000094</a>	
JRCNM10404	ENM_9000093 <a href="http://purl.enanomapper.org/onto/ENM_9000093">http://purl.enanomapper.org/onto/ENM_9000093</a>	
JRCNM62001a	ENM_9000095 <a href="http://purl.enanomapper.org/onto/ENM_9000095">http://purl.enanomapper.org/onto/ENM_9000095</a>	
JRCNM62002a	ENM_9000096 <a href="http://purl.enanomapper.org/onto/ENM_9000096">http://purl.enanomapper.org/onto/ENM_9000096</a>	
JRCNM62101a	ENM_9000079 <a href="http://purl.enanomapper.org/onto/ENM_9000079">http://purl.enanomapper.org/onto/ENM_9000079</a>	



# F2: rich metadata

## Nano safety data



The screenshot shows the eNanoMapper NANoREG database search results page. The browser address bar displays <https://search.data.enanomapper.net/nanoreg/>. The page features a navigation bar with links to Home, Search, Data collections, Data templates, and Help. A search bar is located on the right side of the navigation bar. On the left, there is a sidebar with filters for Data sources (22926), Nanomaterial type (22926), and TOX (15330). The main content area displays a list of search results under the 'Hits list' tab. The first two results are:

- Ag @ IIT (Ag 20 nm) silver nanoparticle**  
CORE (1): ...  
Results: P-CHEM. Particle size distribution (Granulometry)  
[more](#)  
[Material](#) [Composition](#) [Studies](#) [Add to Selection](#)
- Au@PBPK (Au 13 nm) gold nanoparticle**  
CORE (1): ...  
Results: P-CHEM. Specific surface area, P-CHEM. Particle size distribution (Granulometry)  
[more](#)  
[Material](#) [Composition](#) [Studies](#) [Add to Selection](#)

The third result is partially visible: **CeO2@PBPK (CeO2 140-200 nm) cerium oxide nanoparticle**.



# F3: registered or indexed



Home

eNanoMapper

NANoREG

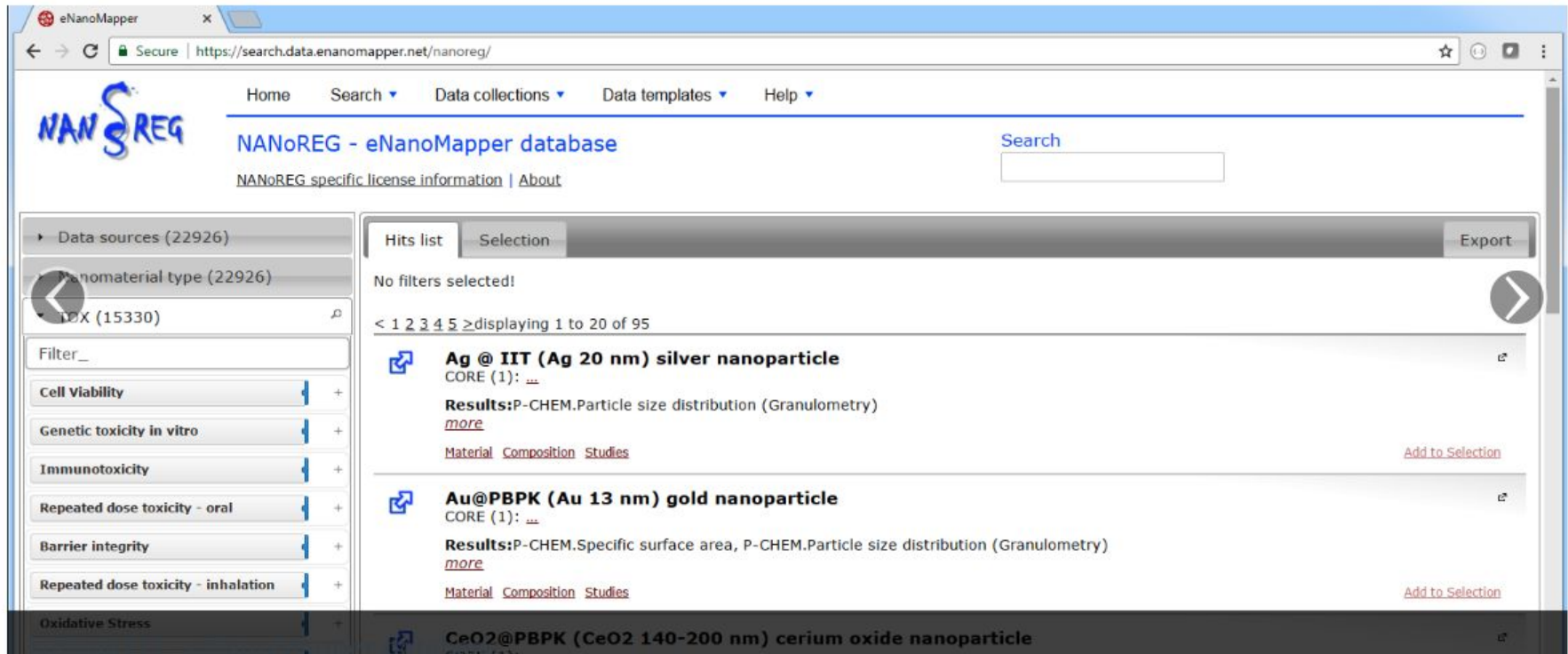
NanoReg2

caLIBRAte

GRACIOUS

PATROLS

## Nano safety data



The screenshot shows the eNanoMapper web application interface. The browser address bar displays the URL <https://search.data.enanomapper.net/nanoreg/>. The page header includes navigation links: Home, Search, Data collections, Data templates, and Help. The main content area is titled "NANoREG - eNanoMapper database" and features a search bar. On the left, a sidebar lists data sources (22926) and filters, including Nanomaterial type (22926), TOX (15330), and various toxicity endpoints like Cell Viability, Genetic toxicity in vitro, Immunotoxicity, Repeated dose toxicity - oral, Barrier integrity, Repeated dose toxicity - inhalation, and Oxidative Stress. The main results area shows a "Hits list" with "No filters selected!" and "displaying 1 to 20 of 95" results. The first two results are:

- Ag @ IIT (Ag 20 nm) silver nanoparticle**  
CORE (1): ...  
Results: P-CHEM. Particle size distribution (Granulometry)  
[more](#)  
[Material](#) [Composition](#) [Studies](#) [Add to Selection](#)
- Au@PBPk (Au 13 nm) gold nanoparticle**  
CORE (1): ...  
Results: P-CHEM. Specific surface area, P-CHEM. Particle size distribution (Granulometry)  
[more](#)  
[Material](#) [Composition](#) [Studies](#) [Add to Selection](#)

The third result is partially visible: **CeO2@PBPk (CeO2 140-200 nm) cerium oxide nanoparticle**.



# eNanoMapper → EU Observatory for Nano



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English (en) ▼



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## Have your say on future studies on nanomaterials

14 January 2019

The EUON conducts up to 3 studies annually. They aim to address knowledge gaps relating to nanomaterials that are of interest to the general public and the research community. The EUON is now looking for topic suggestions that could be addressed in its upcoming studies.

[More news](#) | [RSS](#)

News



Maastricht University

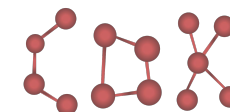
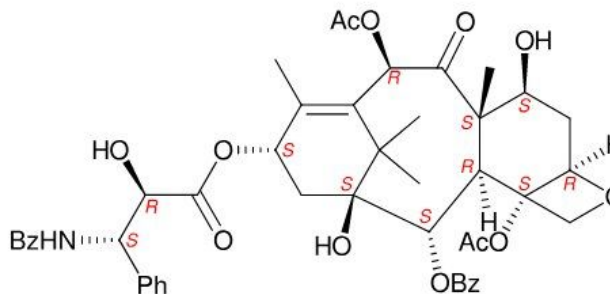
Logo's: all rights reserved.  
(claiming fair use)



# Wikidata + Scholia: encyclopedia

## paclitaxel (Q423762)

Paclitaxel (PTX), sold under the brand name Taxol among others, is a chemotherapy medication used to treat a number of types of cancer. This includes ovarian cancer, breast cancer, lung cancer, Kaposi sarcoma, cervical cancer, and pancreatic cancer. It is given by injection into a vein. ... (from the [English Wikipedia](#))



## Identifiers

Show  entries

Search:

IDpred	Id
<a href="#">ATC code</a>	L01CD01
<a href="#">CAS Registry Number</a>	33069-62-4

Show  entries

Search:

Mol	InChIKey	CAS	ChemSpider	PubChem CID
<a href="#">acetic acid</a>	QTBSBXVTEAMEQO-UHFFFAOYSA-N	64-19-7	171	176
<a href="#">deuterated acetic acid</a>	QTBSBXVTEAMEQO-GUEYOVJQSA-N	1186-52-3	2006083	2723903
<a href="#">acetic acid c-14</a>	QTBSBXVTEAMEQO-HQMMQRPASA-N	2845-03-6	144444	164769
<a href="#">acetic acid c-13</a>	QTBSBXVTEAMEQO-VQEHIDDOSA-N	1563-79-7	8329490	10153982
<a href="#">acetic acid c-11</a>	QTBSBXVTEAMEQO-JVVVGQRLSA-N	78887-71-5	396653	450349
<a href="#">acetate ion</a>	QTBSBXVTEAMEQO-UHFFFAOYSA-M	71-50-1	170	175

[Edit on query.Wikidata.org](#)

Showing 1 to 6 of 6 entries



Maastricht University



Previous

1

Next



# A1: standard protocols

HTTP, REST/OpenAPI, BioSchemas,  
RDF, SPARQL, ...



**OpenRiskNet**  
RISK ASSESSMENT E-INFRASTRUCTURE

## eNanoMapper database

The eNanoMapper prototype database is part of the computational infrastructure for toxicological data management of engineered nanomaterials, developed within the EU FP7 eNanoMapper project. Provides support for upload, search and ...

Provided by: Maastricht University  
Type: Database / data source  
Applicability domain: Toxicology, Bioinformatics  
Topic: Information extraction, Nano safety, Chemical properties

- ✓ For end-users
- ✓ For developers

[DETAILS →](#) [VISIT SERVICE →](#)

## AOP-Wiki SPARQL Endpoint

This service is a Virtuoso SPARQL endpoint that is loaded with RDF of the Adverse Outcome Pathway (AOP)-Wiki database (<https://aopwiki.org/>), based on the quarterly XML dumps that ...

Provided by: Maastricht University  
Type: Database / data source  
Applicability domain: Toxicology, Bioinformatics  
Topic: Information extraction, Risk assessment

- ✓ For end-users
- ✓ For developers



[DETAILS →](#)

## WikiPathways SPARQL Endpoint

WikiPathways was established to facilitate the contribution and maintenance of pathway information by the biology community. WikiPathways is an open, collaborative platform dedicated to the curation of biological pathways. WikiPathways ...

Provided by: Maastricht University  
Type: Database / data source  
Applicability domain: Bioinformatics  
Topic: Information extraction  
Biological area: Acute toxicity, Carcinogenicity, Mutagenicity, Genotoxicity, Skin sensitisation, Omics, Transcriptomics

- ✓ For end-users
- ✓ For developers

[DETAILS →](#) [VISIT SERVICE →](#)

## BridgeDb identifier mapping service (Homo sapiens, Mus musculus and Rattus norvegicus)

BridgeDb is a platform for database identifier mapping, both simple identifiers (e.g. CHEBI:1234) and universal resource identifiers (URIs, e.g. <http://identifiers.org/chebi/CHEBI:1234>). It is ...





Provided by: Maastricht University  
Type: Database / data source, Service  
Applicability domain: Bioinformatics  
Topic: Identifier mapping

- ✓ For developers
- ✓ For end-users

[DETAILS →](#) [VISIT SERVICE →](#)



# BioSchema: Datasets

Property	Expected Type	Description	CD	Controlled Vocabulary	Example
<b>Marginality: Minimum.</b>					
<u><b>description</b></u>	<u>Text</u>	<p><b>Schema:</b> A description of the item.</p> <p><b>Bioschemas:</b> A short summary describing a dataset.</p>	ONE		
<u><b>identifier</b></u>	<u>PropertyValue</u> <u>Text</u> <u>URL</u>	<p><b>Schema:</b> The identifier property represents any kind of identifier for any kind of Thing, such as ISBNs, GTIN codes, UUIDs etc. Schema.org provides dedicated properties for representing many of these, either as textual strings or as URL (URI) links. See <u><a href="#">background notes</a></u> for more details.</p>	MANY		
<u><b>keywords</b></u>	<u>Text</u>	<p><b>Schema:</b> Keywords or tags used to describe this content. Multiple entries in a keywords list are typically delimited by commas.</p> <p><b>Bioschemas:</b> These keywords provide a summary of the dataset.</p>	MANY		
<u><b>name</b></u>	<u>Text</u>	<p><b>Schema:</b> The name of the item.</p> <p><b>Bioschemas:</b> A descriptive name of the dataset.</p>	ONE		

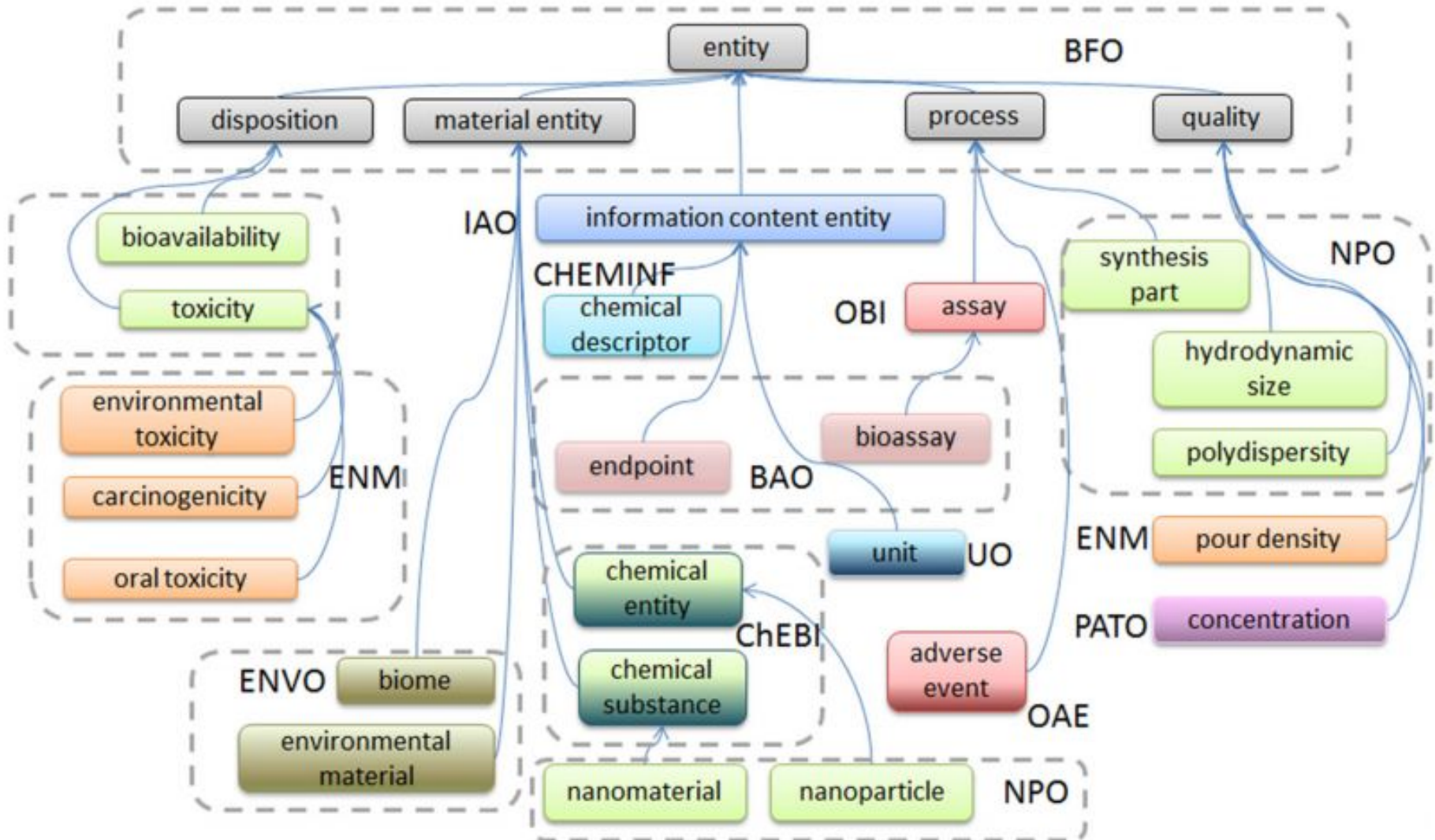


# BioSchema: Chemical Substances

Property	Expected Type	Description
Properties from <a href="#">ChemicalSubstance</a> (pending schema.org integration).		
<b>molecularFormula</b>	<a href="#">Text</a>	The empirical formula is the simplest whole number ratio of all the atoms in a molecule.
<b>biochemicalInteraction</b>	<a href="#">BioChemEntity</a>	A BioChemEntity that is known to interact with the item.
<b>biochemicalSimilarity</b>	<a href="#">BioChemEntity</a>	A similar molecular substance or molecular entity, e.g., obtained by fingerprint similarity algorithms.
<b>biologicalRole</b>	<a href="#">DefinedTerm</a>	A role played by the molecular entity within a biological context.
<b>chemicalRole</b>	<a href="#">DefinedTerm</a>	A role played by the molecular entity within a chemical context.
<b>potentialUse</b>	<a href="#">DefinedTerm</a>	Intended use of the molecular entity by humans.
Properties from <a href="#">BioChemEntity</a>		
<b><a href="#">additionalProperty</a></b>	<a href="#">PropertyValue</a>	A property-value pair representing an additional characteristics of the entity, e.g. a product feature (e.g. <a href="#">http://schema.org/brand</a> ) matching property in schema.org. Note: Publishers should be aware that applications designed to use specific schema.org properties (e.g. <a href="#">http://schema.org/gtin13</a> , ...) will typically expect such data to be provided using those properties, rather than this property.
<b>associatedDisease</b>	<a href="#">MedicalCondition</a> or <a href="#">URL</a>	Disease associated to this BioChemEntity.



# I1: common language







RESEARCH

Open Access

# eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment

Janna Hastings<sup>1\*</sup>, Nina Jeliazkova<sup>2</sup>, Gareth Owen<sup>1</sup>, Georgia Tsiliki<sup>3</sup>, Cristian R Munteanu<sup>4,5</sup>, Christoph Steinbeck<sup>1</sup> and Egon Willighagen<sup>5</sup>

## Abstract

Engineered nanomaterials (ENMs) are being developed to meet specific application needs in diverse domains across the engineering and biomedical sciences (e.g. drug delivery). However, accompanying the exciting proliferation of novel nanomaterials is a challenging race to understand and predict their possibly detrimental effects on human health and the environment. The eNanoMapper project ([www.enanomapper.net](http://www.enanomapper.net)) is creating a pan-European computational infrastructure for toxicological data management for ENMs, based on semantic web standards and ontologies. Here, we describe the development of the eNanoMapper ontology based on adopting and extending



# Ontologies define hierarchies (also)

## metal oxide nanoparticle

- aluminium oxide nanoparticle
- cadmium(II) oxide nanoparticle
- cerium oxide nanoparticle
- copper oxide nanoparticle
- copper(II) oxide nanoparticle
- europium trioxide nanoparticle
- iron oxide nanoparticle
  - dextran-coated iron oxide nanoparticle
  - hematite nanoparticle
  - iron (II,III) oxide nanoparticle
  - iron (III) oxide nanoparticle
  - magnetite nanoparticle
  - superparamagnetic iron oxide nanoparticle
- manganese (IV) dioxide nanoparticle
- molybdenum trioxide nanoparticle

- transferase activity assay

## gene expression assay

- reporter gene assay
- transcriptional response profiling assay

## genotoxicity assay

- DNA Damage Assay
- ion channel assay
- localization assay
- membrane potential assay
  - ion channel assay
  - mitochondrial membrane potential assay
  - nuclear membrane potential assay
  - plasma membrane potential assay
- metastasis assay
- organism behavior assay



# All metal oxides showing genotoxicity

Which metal oxides (*NPO\_1541*) show a form of genotoxicity (*BAO\_0002167*)?

substance	particleType	experiment	protocol	value	unit
Gerloff2009 NM2	titanium oxide nanoparticle	DNA in Tail	Fpg-2Dmodified Comet Assay	6.0	%
Gerloff2009 NM2	titanium oxide nanoparticle	DNA in Tail	Fpg-2Dmodified Comet Assay	5.0	%
Gerloff2009 NM2	titanium oxide nanoparticle	DNA in Tail	Fpg-2Dmodified Comet Assay	8.0	%
Gerloff2009 NM2	titanium oxide nanoparticle	DNA in Tail	Fpg-2Dmodified Comet Assay	3.0	%
TiO2	titanium oxide nanoparticle	DNA in Tail	Fpg-2Dmodified Comet Assay	6.0	%
TiO2	titanium oxide nanoparticle	DNA in Tail	Fpg-2Dmodified Comet Assay	5.0	%
TiO2	titanium oxide nanoparticle	DNA in Tail	Fpg-2Dmodified Comet Assay	8.0	%
TiO2	titanium oxide nanoparticle	DNA in Tail	Fpg-2Dmodified Comet Assay	3.0	%
ZnO	zinc oxide nanoparticle	DNA in Tail	Fpg-2Dmodified Comet Assay	23.0	%



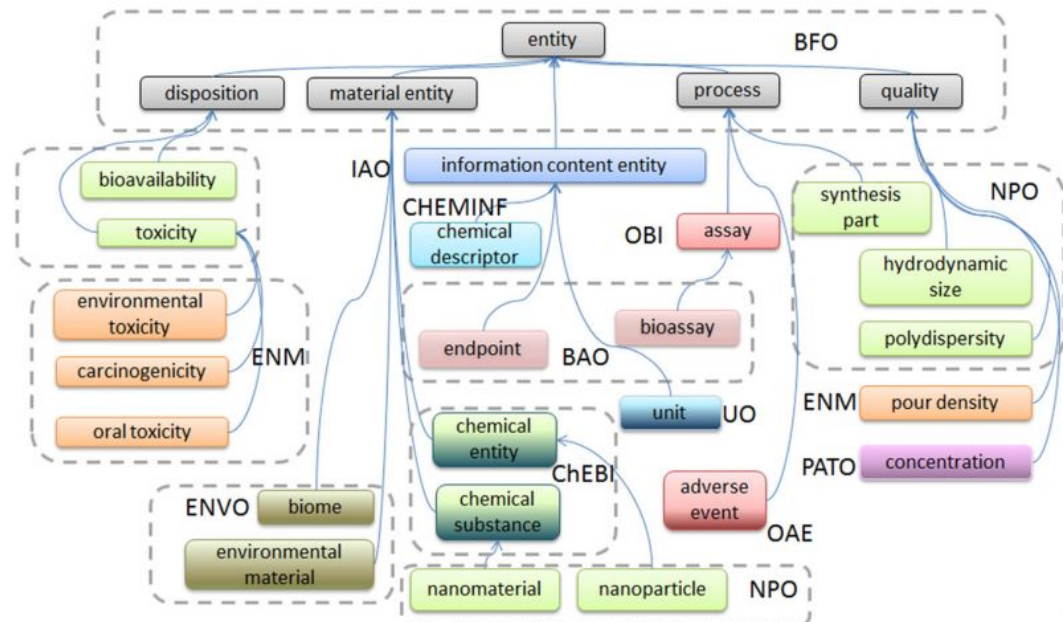
# I2: FAIR vocabularies

F1: identifiers, F2: rich metadata, F3: registered or indexed, F4: specify identifiers

A1: standard protocols, A2: metadata persistent

I1: common language, I2: FAIR vocabularies, I3: references other FAIR

R1: clear license, provenance, community standards



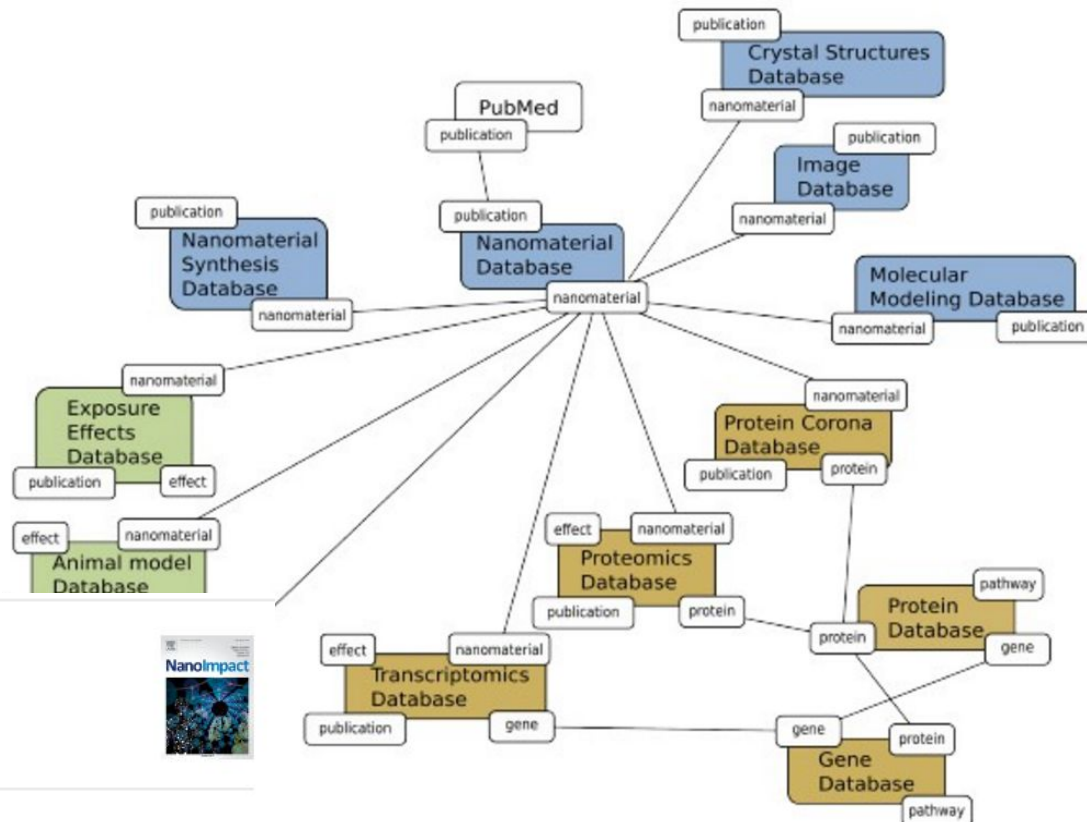


# I3: references other FAIR





# Linked (Open) Data



NanoImpact

Volume 9, January 2018, Pages 85-101



Research paper

## Integration among databases and data sets to support productive nanotechnology: Challenges and recommendations

Sandra Karcher<sup>a, q</sup>, Egon L. Willighagen<sup>b</sup>, John Rumble<sup>c, d</sup>, Friederike Ehrhart<sup>b</sup>, Chris T. Evelo<sup>b</sup>, Martin Fritts<sup>e</sup>, Sharon Gaheen<sup>e</sup>, Stacey L. Harper<sup>f</sup>, Mark D. Hoover<sup>g</sup>, Nina Jeliaskova<sup>h</sup>, Nastassja Lewinski<sup>i</sup>, Richard L. Marchese Robinson<sup>j, k, l, 2</sup>, Karmann C. Mills<sup>l</sup>, Axel P. Mustad<sup>m</sup>, Dennis G. Thomas<sup>n</sup>, Georgia Tsiliki<sup>o, p</sup>, Christine Ogilvie Hendren<sup>q, r, s</sup>

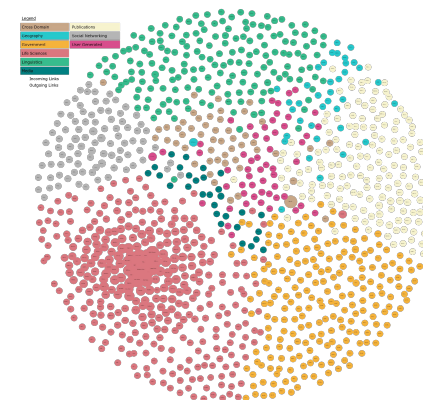
Show more

<https://doi.org/10.1016/j.impact.2017.11.002>

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"Linking Open Data cloud diagram 2017, by Andrejs Abele, John P. McCrae, Paul Buitelaar, Anja Jentzsch and Richard Cyganiak. <http://lod-cloud.net/>"



# R1: clear license, provenance, community standards



Home Search ▼ Data collections ▼ Data upload ▼ For developers

Home > All assessments > This assessment > Versions >

Assessment identifier

Collect structures

Endpoint data used

Assessment details

Title* ⓘ:	NanoWiki
Maintainer* ⓘ:	<a href="http://orcid.org/0000-0001-7542-0286">http://orcid.org/0000-0001-7542-0286</a>
Purpose* ⓘ:	Nanomaterials, physicochemical characterisations and toxicity data, imported via NanoWiki RDF dump
Version ⓘ:	2
Version start date ⓘ:	14.03.2016
Version last modified on ⓘ:	14.03.2016
Status ⓘ:	Final Assessment
License*:	<a href="https://creativecommons.org/publicdomain/zero/1.0/">https://creativecommons.org/publicdomain/zero/1.0/</a>
Rights holder* ⓘ:	<a href="http://orcid.org/0000-0001-7542-0286">http://orcid.org/0000-0001-7542-0286</a>
See also* ⓘ:	NanoWiki
Source URL* ⓘ:	<a href="http://dx.doi.org/10.6084/m9.figshare.1330208">http://dx.doi.org/10.6084/m9.figshare.1330208</a>
Identifier ⓘ:	00000000-0000-0000-0000-000000000001
Rating ⓘ:	★★★★★☆☆☆☆

```
:chembl_rdf_dataset a void:Dataset ;
>> dcterms:title "The ChEMBL Database" ;
>> dcterms:description "ChEMBL is a database of bioac
>> structures, calculated properties (e.g. logP, Mole
>> bioactivities (e.g. binding constants, pharmacolog
>> from the primary scientific literature, and cover
>> modern drugs." ;
>> pav:createdBy <http://orcid.org/0000-0002-8011-030
>> pav:createdOn "2009-10-28T00:00:00.000Z"^^xsd:date
>> pav:lastUpdateOn "2013-05-07T00:00:00.000+01:00"^^
>> dcterms:issued "2013-08-23T00:00:00.000+01:00"^^xs
>> pav:version "16.example" ;
>> pav:previousVersion <http://rdf.ebi.ac.uk/dataset/
>> dcat:landingPage <https://www.ebi.ac.uk/chembl> ;
>> foaf:page <ftp://ftp.ebi.ac.uk/pub/databases/chemb
```

Open PHACTS Working Draft



Dataset Descriptions for the Open Pharmacological Space

Open PHACTS Working Draft 12 September 2013

This version:

<http://www.openphacts.org/specs/2013/WD-datadesc-20130912/>

Latest published version:

<http://www.openphacts.org/specs/datadesc/>

Previous version:

<http://www.openphacts.org/specs/2012/WD-datadesc-20121019/>

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Maastricht University



Bioschemas



# R1: clear license, provenance, community standards



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# Collaborative research: about licensing, waiving, and ownership

Research article

Bioinformatics

Ethical Issues

Legal Issues

Egon Willighagen 

January 26, 2017

> Author and article information

▼ Abstract

Research collaborations are hampered by copyright law. While these laws are aimed at solving sustainability of writing and later other creative processes, and nowadays knowledge too, they make it harder in a time where research is funded with on temporary projects. This article discusses some of the aspects involved, though the legal foundations are only minimally brought up. One critical aspect is the role of consortium agreements. It also



# Gaps



F4: specify identifiers

A2: metadata persistent

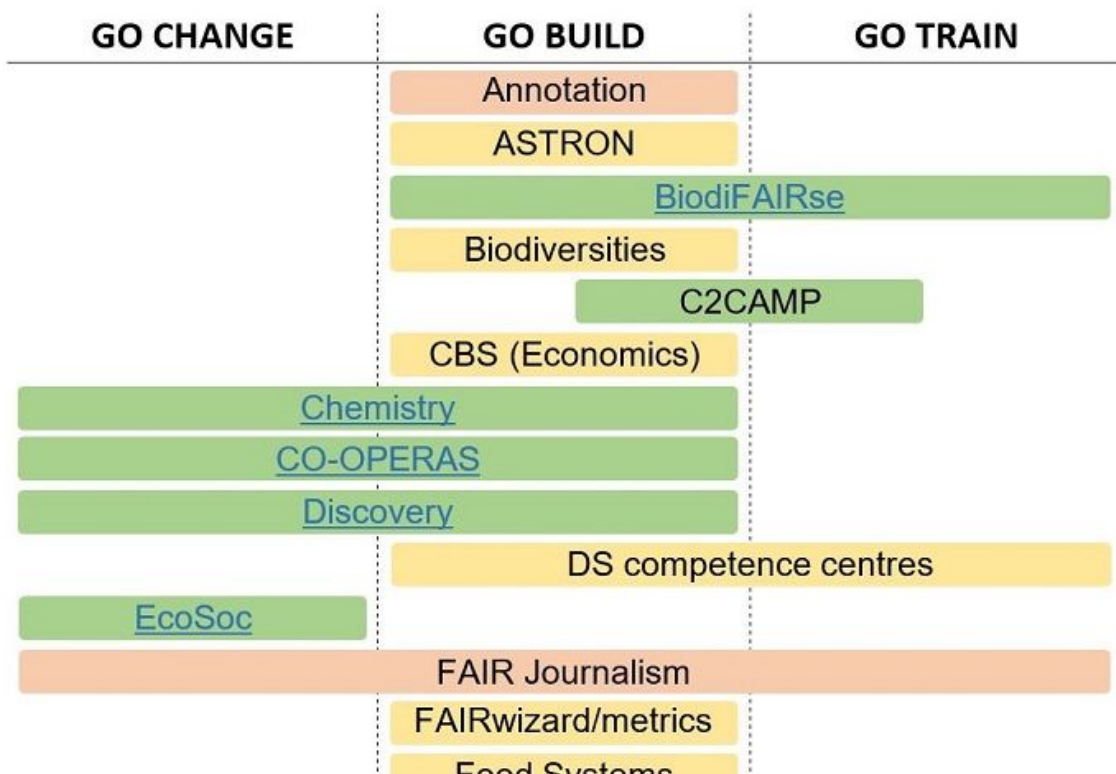
I1: common language, I2: FAIR vocabularies, I3:  
references other FAIR

*R1: clear license, provenance*



# GO FAIR Chemistry Implementation

## Network



**F**indable   
**A**ccessible   
**I**nteroperable   
**R**eusable 

SCIENTIFIC DATA

Comment | [OPEN](#) | Published: 26 June 2018

## A design framework and exemplar metrics for FAIRness

Mark D. Wilkinson , Susanna-Assunta Sansone , Erik Schultes, Peter Doorn, Luiz Olavo Bonino da Silva Santos & Michel Dumontier 

Scientific Data **5**, Article number: 180118 (2018) | [Download Citation](#) ↓



# ELIXIR Toxicology Community

egonw / ELIXIR-Tox

Unwatch ▾

11

★ Star

0

🔗 Fork

1

<> Code

🔔 Issues 14

🔗 Pull requests 0

📁 Projects 7

📊 Insights

⚙️ Settings

Filters ▾

🔍 is:issue is:open

🏷️ Labels 14

📅 Milestones 2

New issue

📁 14 Open ✓ 12 Closed

Author ▾

Projects ▾

Labels ▾

Milestones ▾

Assignee ▾

Sort ▾

📁 🟢 reboot/boost of the process task

#27 opened a day ago by egonw



4

📁 🟢 reach out to EPA CompTox Dashboard for BioSchemas annotation

#26 opened on Nov 29, 2018 by egonw

📁 🟢 make BioSchemas annotation for substances like nanomaterials BioSchemas NanoCommons



OpenRiskNet task

#25 opened on Nov 29, 2018 by egonw

📁 🟢 Create Turtle file of AOP Wiki XML EU-ToxRisk OpenRiskNet

#24 opened on Aug 8, 2018 by marvinm2



3

📁 🟢 establish contact with teh NSC WG A on dissemination and training NanoCommons TeSS task

#23 opened on Jun 14, 2018 by egonw



1



Maastricht University





## Toxicology data management tutorials automatically collected by European training portal TeSS

Posted on [19 July 2018](#)

**A team including Egon Willighagen from Maastricht University, Niall Beard from ELIXIR's TeSS team, and Oana Florean from Douglas Connect (coordinator of OpenRiskNet) has used BioSchemas to create a system that automatically pulls toxicology-related training materials from the eNanoMapper project into the European training portal TeSS.**

**TeSS** is ELIXIR's training portal. It provides trainers and trainees with training materials, events and interactive tutorials in the field of life sciences. Egon Willighagen: "The toxicology training materials that we have now added to TeSS originate from the eNanoMapper project. This FP7 project developed a computational infrastructure for toxicology data management of engineered nanomaterials. Within eNanoMapper, we developed **many tutorials**. In the beginning, we put these online in Microsoft Word format. At a certain point, our Programme Technical Officer Cedric Notredame from Spain pushed us to make the training resources available in a more sustainable, machine-readable format. However, we did not have enough time to do this within the eNanoMapper project."

### Machine-readable

Willighagen continues: "Now, we have started two new European toxicology projects (OpenRiskNet and NanoCommons). In addition, we are developing a proposal for an ELIXIR Toxicology Community. So, I really wanted to make the tutorials available to a larger audience. I asked on Twitter if people knew how to use BioSchemas to this end. Niall Beard from ELIXIR's TeSS team replied that he had some ideas. That same afternoon, he sent me a pull request on Github with BioSchemas annotations."

The TeSS team can write scripts ('scrapers') to eNanoMapper website. The scrapers run and the team can create a scraper as long as the target is about the tutorials," says Willighagen.

### Bioschemas

**Bioschemas** encourages people to use schema.org extensive library of simple, lightweight schemas to improve search engine visibility and interoperability. For instance, 'Event' is a type that has properties like 'start date'. Schema.org extensions with life science vocabularies. This all makes it easier to discover

  
**eNanoMapper**  
 eNanoMapper developed a computational infrastructure for toxicological data management of...  
**9 training materials**
  
**OpenRiskNet**  
 The main objective of OpenRiskNet is to develop an open e-Infrastructure providing resources and...  
**0 upcoming events (2 past events)**
  
**BiGCaT**  
 Department of Bioinformatics - BiGCaT, Maastricht University  
 The department of Bioinformatics-BiGCaT is part of NUTRIM the school of Nutrition and...  
**5 training materials**  
**0 upcoming events (1 past event)**
  
**NanoCommons**  
 NanoCommons will deliver a sustainable and openly accessible nanoinformatics framework...  
**1 training material**  
**0 upcoming events (1 past event)**


**NanoCommons**

Nano-Knowledge Community



**OpenRiskNet**  
RISK ASSESSMENT E-INFRASTRUCTURE



# Summarizing

1. NanoSafety Cluster (“eNanoMapper”) already pretty FAIR
2. Gaps
3. Synergy with ELIXIR, GO FAIR
4. EU NanoSafety Cluster / US NanoWG
  - Working Groups, US-EU CoRs
  - NanoCommons, OpenRiskNet, EU-ToxRisk
  - Gov4Nano, RiskGONE, NANORIGO
  - NanoSolveIT, NanoInformaTIX



# NanoCommons Transnational Access

## Transnational access

The NanoCommons Transnational Access (TA) is the ability of nanosafety Researchers from industry, academia and regulatory bodies to access the state-of-the-art NanoCommons expertise free of charge and take advantage of the NanoCommons services, facilities and knowledge to advance their work, solve problems and take their research to the next level.

NanoCommons is designed to provide innovative solutions for decision support tools that require organised high-quality data platform and the supporting tools will be provided to the nano via funded calls for Transnational access, as well as developme

NanoCommons is envisaged as a bridge between academic res recommendations of the NanoSafety Cluster "Closer to the Ma around safety-by-design and Life cycle assessment whilst also i

### Using ontologies to make your research data more FAIR

Using ontologies to make your research data more FAIR Overview Making the most impact with your research, it helps if you had your research data management (RDM) in place. Within the context of the RDM you work on making data more FAIR and perhaps even open, following the requirements from the European Commission. But RDM, FAIR,...

**Read more ▶**

## Access the NanoCommons e-infrastructure

**Transnational Access Guidelines**

**Apply for Transnational Access**

**Transnational Access Services**