FAIR for NanoSafety: where do we stand?

Egon Willighagen
Gov4Nano Kick-off FAIR Workshop
2019-03-06, Den Haag/NL
ORCID: 0000-0001-7542-0286
@egonwillighagen

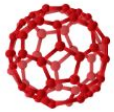
Maastricht University

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

F1: persistent identifiers

eNanoMapper Working Draft



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

Abstract

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

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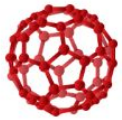
F1: persistent identifiers

eNanoMapper Working Draft



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-EBI

Abstract

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

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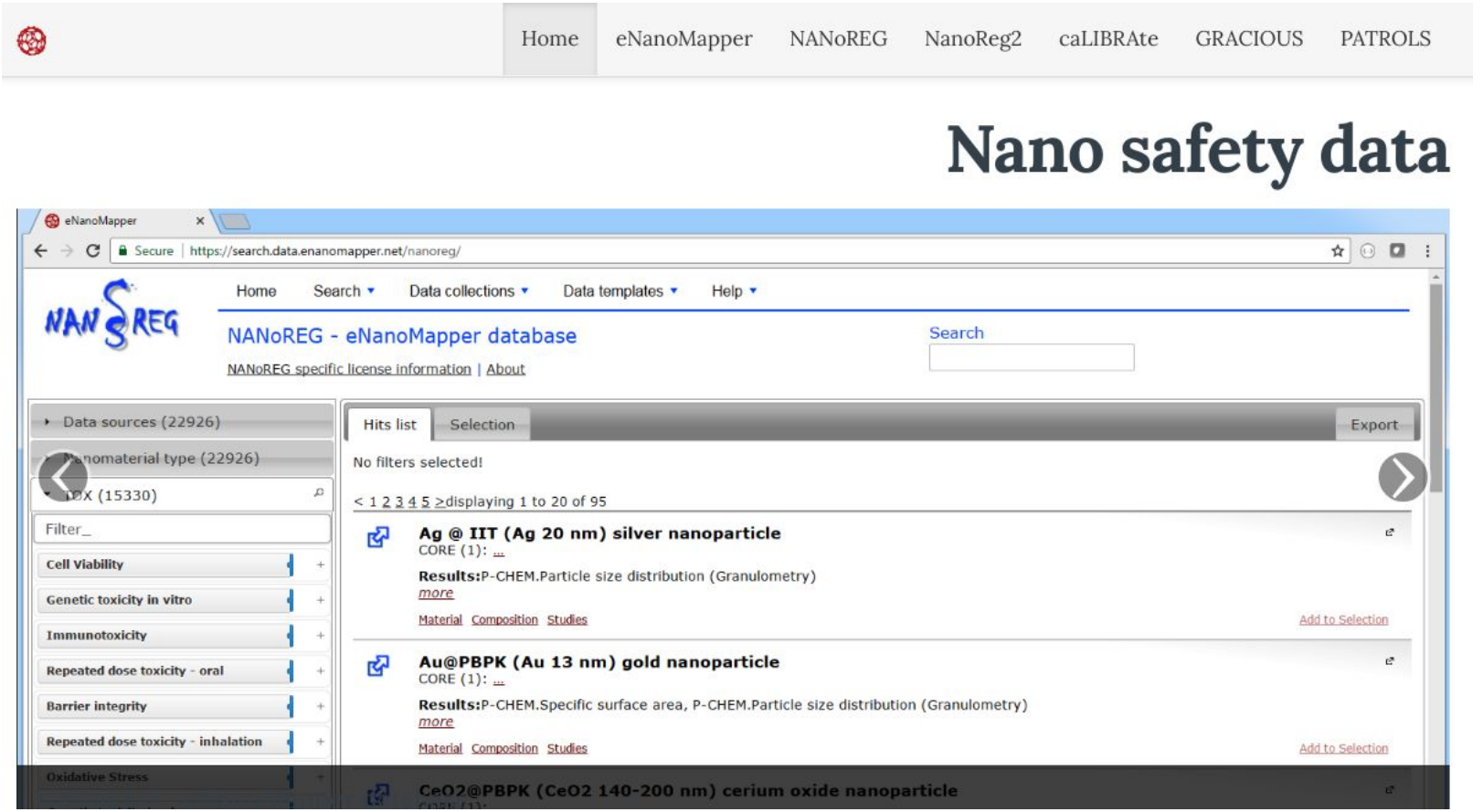
F2: rich metadata



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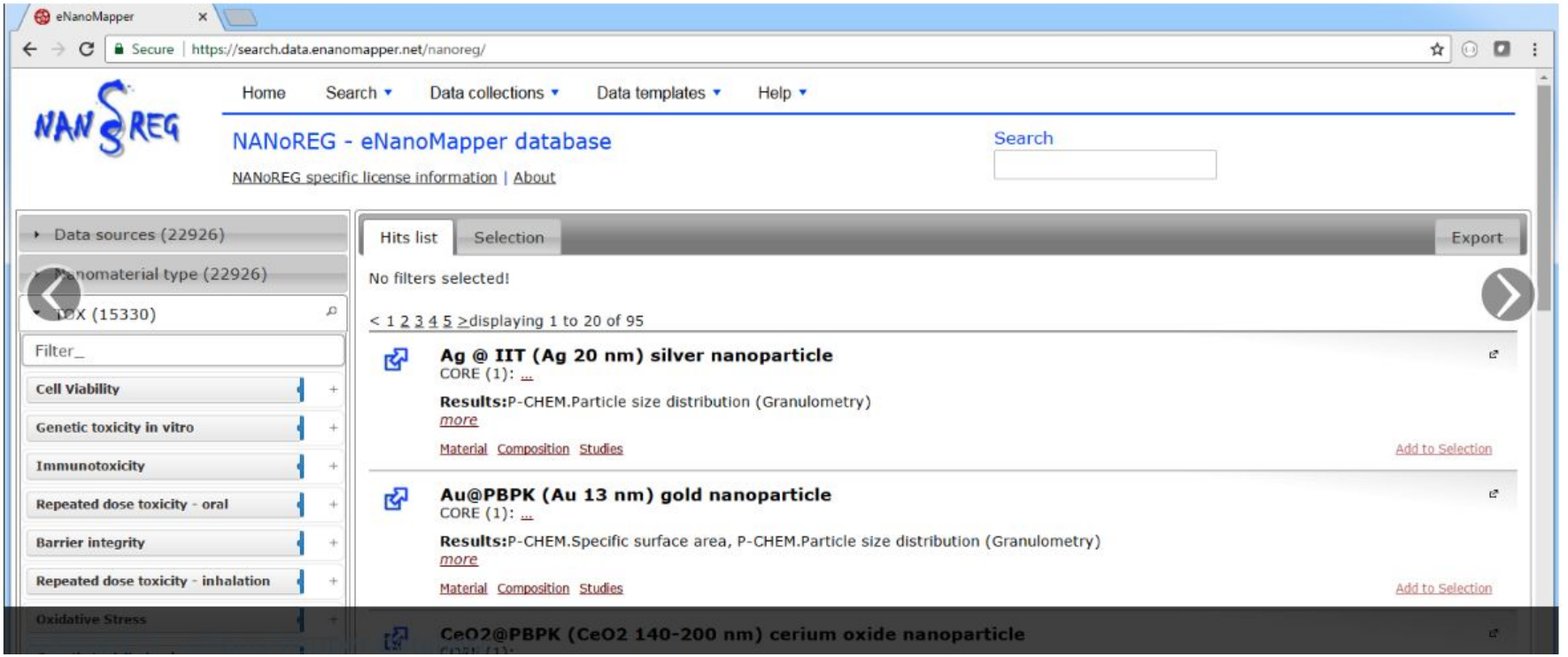
https://data.enanomapper.net/

F3: registered or indexed

NanoSafety Cluster

Home | eNanoMapper | NANoREG | NanoReg2 | caLIBRAte | GRACIOUS | PATROLS

Nano safety data



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https://search.data.enanomapper.net/

eNanoMapper → EU Observatory for Nano

EUON
EUROPEAN UNION OBSERVATORY FOR NANOMATERIALS

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EUROPEAN CHEMICALS AGENCY

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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

NanoData Nano technology knowledge base

eNM eNanoMapper Data and tools for the risk assessment of nanomaterials

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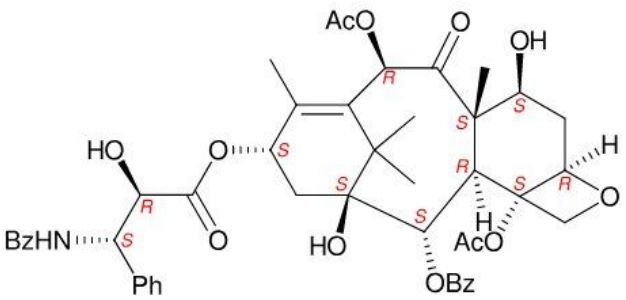
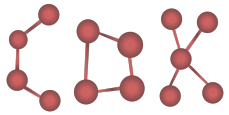
Wikidata + Scholia: encyclopedia

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 10 entries Search:

IDpred	Id
ATC code	L01CD01
CAS Registry Number	33069-62-4

Show 10 entries Search:

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

Edit on query.Wikidata.org

Showing 1 to 6 of 6 entries Previous 1 Next

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A1: standard protocols

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

NanoCommons
Nano-Knowledge Community

OpenRiskNet
RISK ASSESSMENT E-INFRASTRUCTURE

IN PROGRESS

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 →

IN PROGRESS

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

EUTOXRISK

DETAILS →

IN PROGRESS

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 →

IN PROGRESS

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
Marginality: Minimum.					
description	Text	**Schema:** A description of the item. **Bioschemas:** A short summary describing a dataset.	ONE		
identifier	PropertyValue Text URL	**Schema:** 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 background notes for more details.	MANY		
keywords	Text	**Schema:** Keywords or tags used to describe this content. Multiple entries in a keywords list are typically delimited by commas. **Bioschemas:** These keywords provide a summary of the dataset.	MANY		
name	Text	**Schema:** The name of the item. **Bioschemas:** A descriptive name of the dataset.	ONE		

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Bioschemas

elixir

BioSchema: Chemical Substances

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

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Bioschemas

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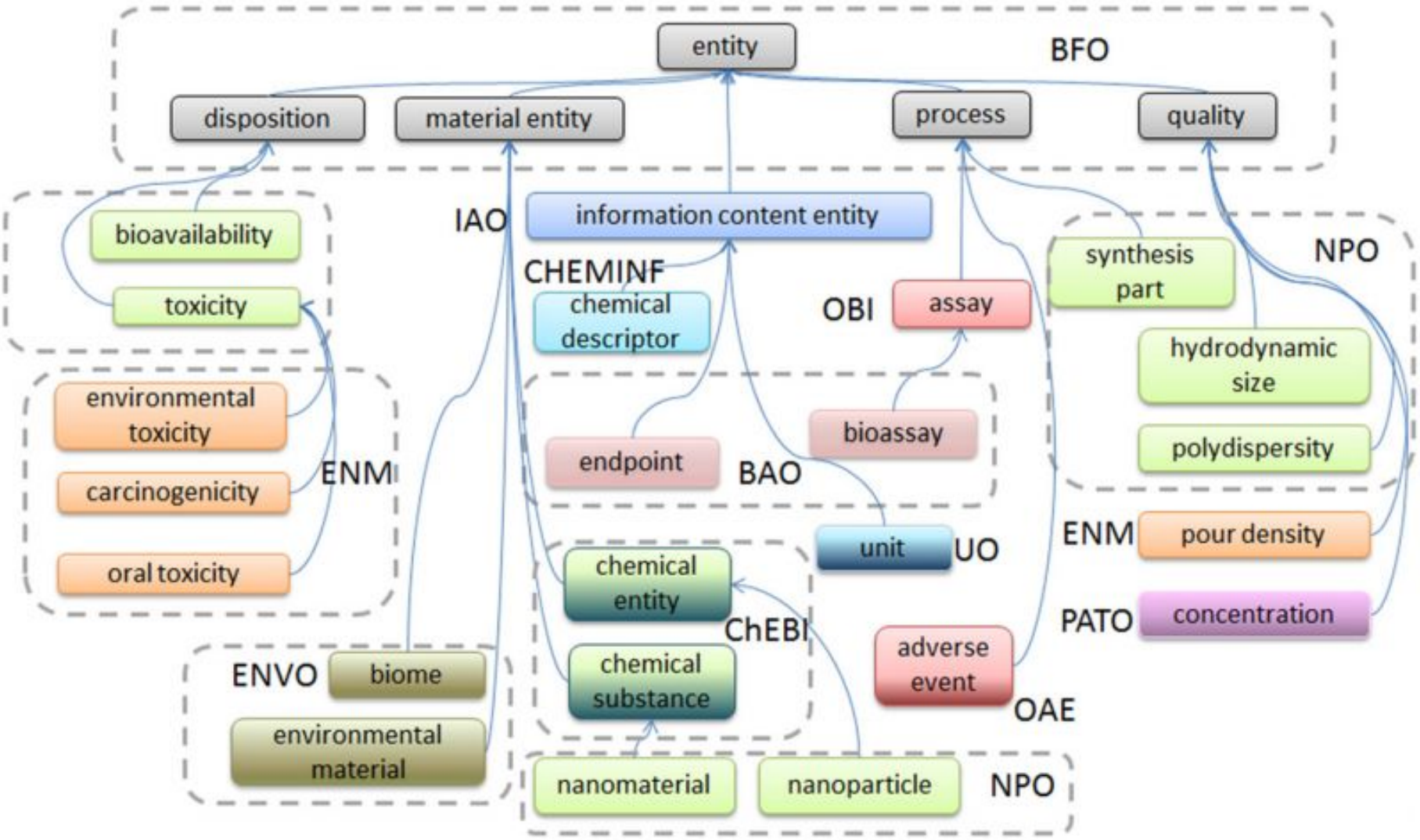
I1: common language



Hastings *et al. Journal of Biomedical Semantics* (2015) 6:10
DOI 10.1186/s13326-015-0005-5

JOURNAL OF BIOMEDICAL SEMANTICS

RESEARCH Open Access

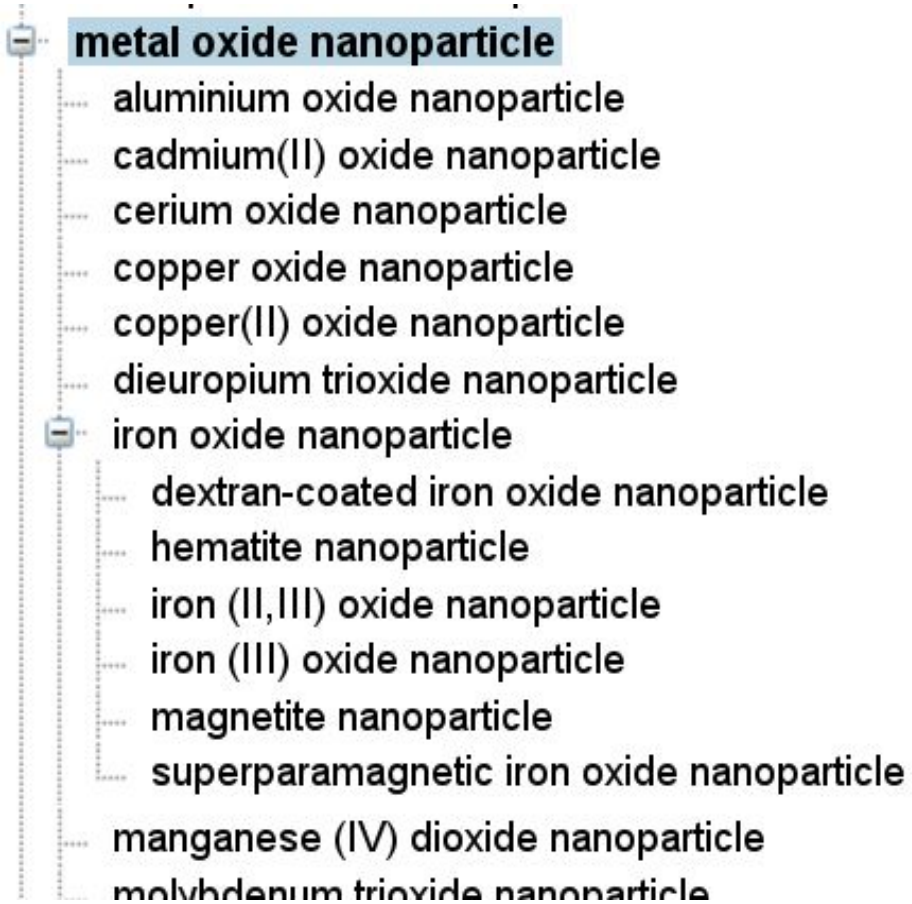
eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment

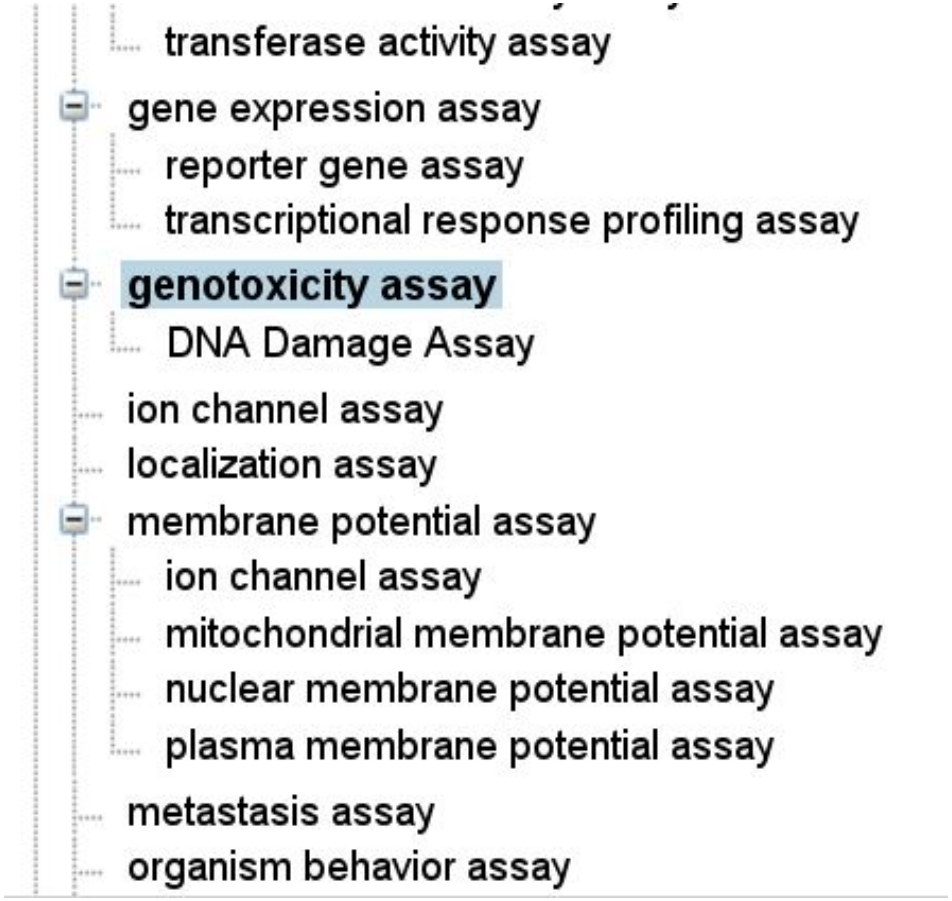
Janna Hastings[1*], Nina Jeliazkova[2], Gareth Owen[1], Georgia Tsiliki[3], Cristian R Munteanu[4,5], Christoph Steinbeck[1] and Egon Willighagen[5]

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) 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)





Hastings *et al. Journal of Biomedical Semantics* (2015) 6:10
DOI 10.1186/s13326-015-0005-5

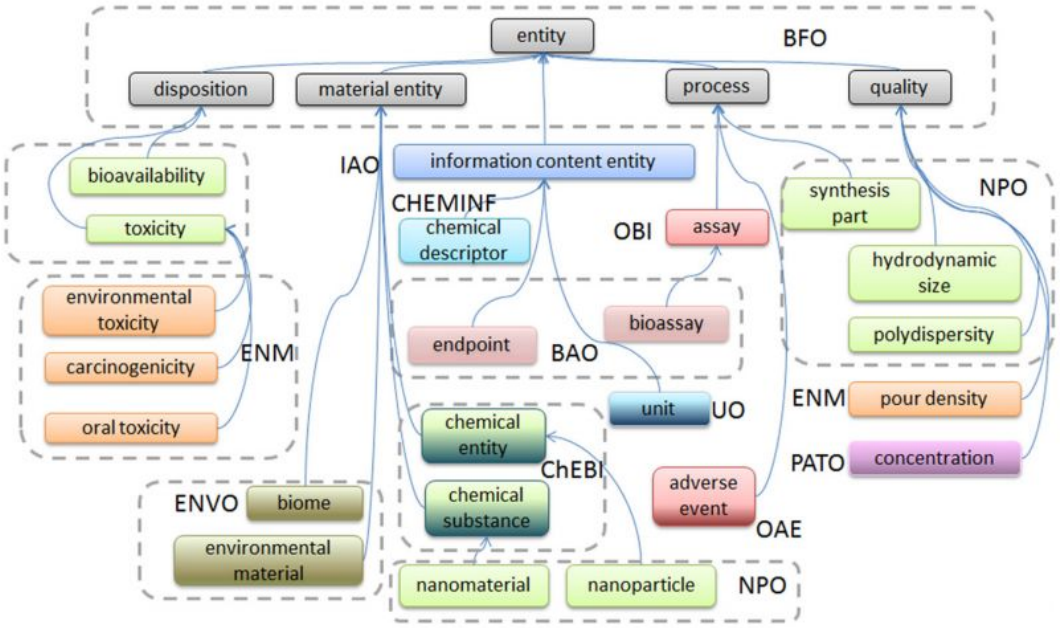
All metal oxides showing genotoxicity

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	%

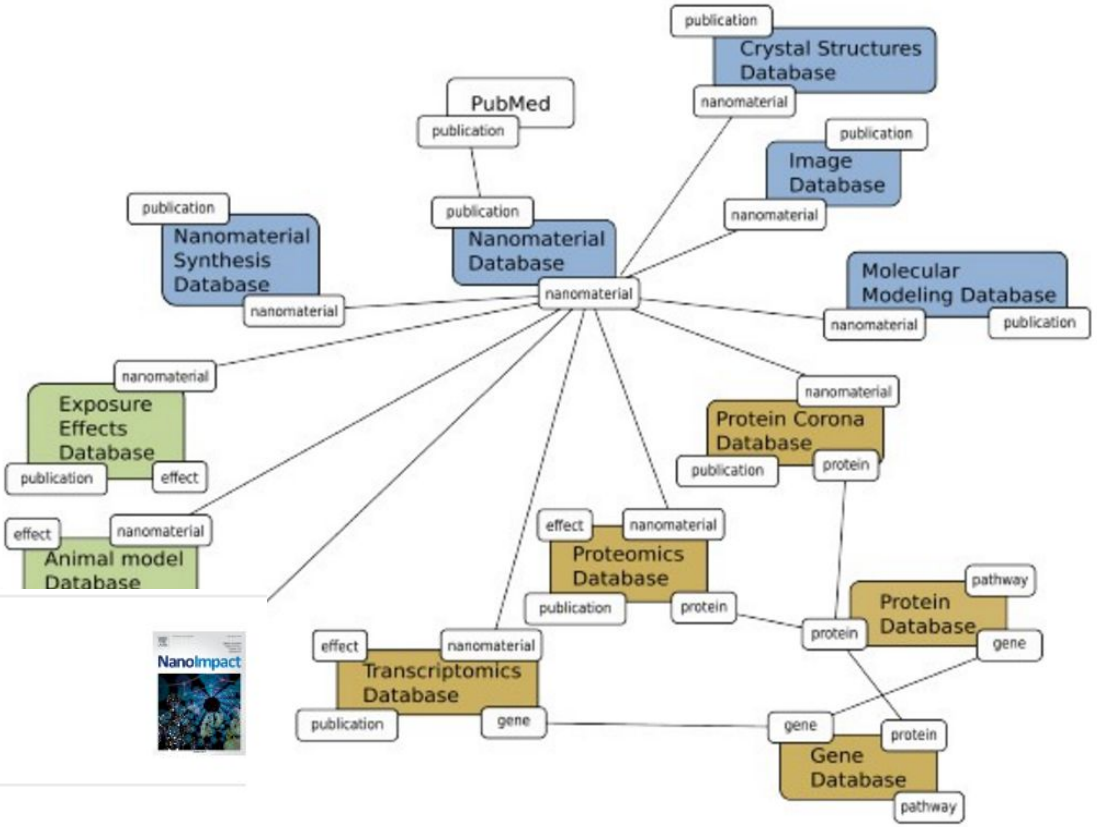
I2: FAIR vocabularies

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



ELSEVIER

NanoImpact

Volume 9, January 2018, Pages 85-101

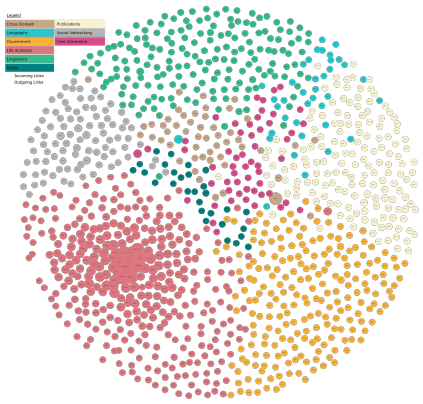
Research paper

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

Sandra Karcher [a, q], Egon L. Willighagen [b], John Rumble [c, d], Friederike Ehrhart [b], Chris T. Evelo [b], Martin Fritts [e], Sharon Gaheen [e], Stacey L. Harper [f], Mark D. Hoover [g], Nina Jeliazkova [h], Nastassja Lewinski [i], Richard L. Marchese Robinson [j, k, 1, 2], Karmann C. Mills [l], Axel P. Mustad [m], Dennis G. Thomas [n], Georgia Tsiliki [o, p], Christine Ogilvie Hendren [q]

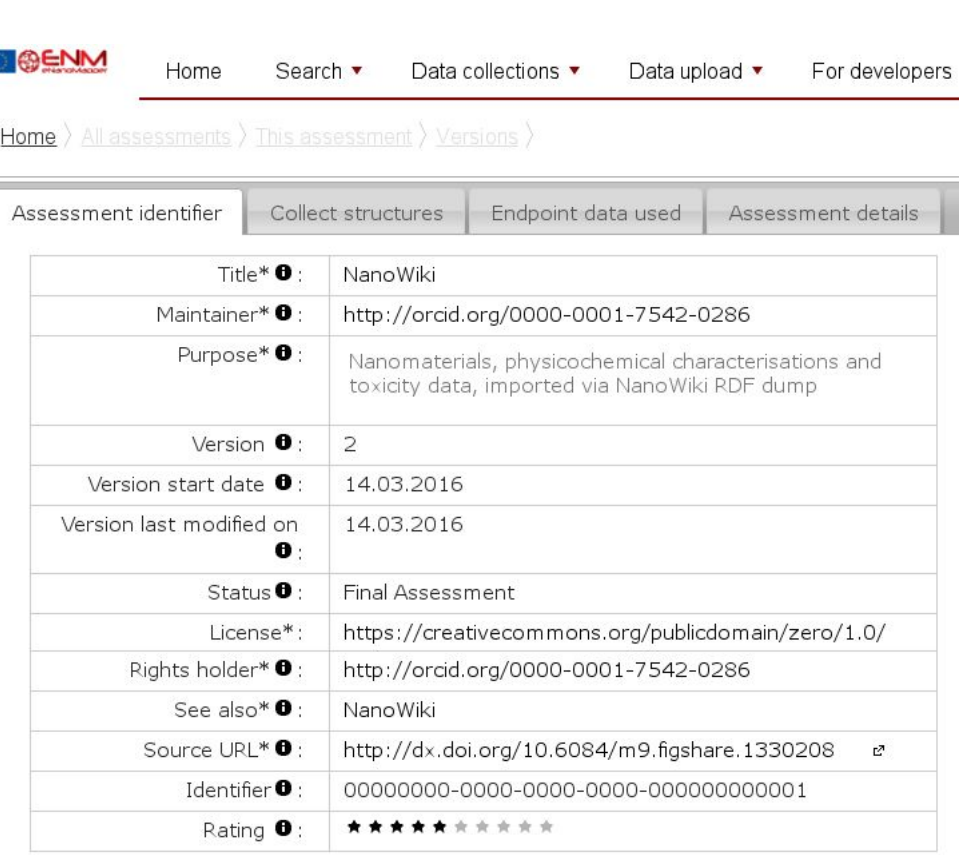
Show more

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



"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




```
: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

Open PHACTS

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/
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Previous version:
http://www.openphacts.org/specs/2012/WD-datadesc-20121019/
Editor:
Alasdair J G Gray, University of Manchester
Authors:
Christian Brenninkmeijer, University of Manchester
Chris Evelo, Maastricht University
Carole Goble, University of Manchester
Alasdair J G Gray, University of Manchester

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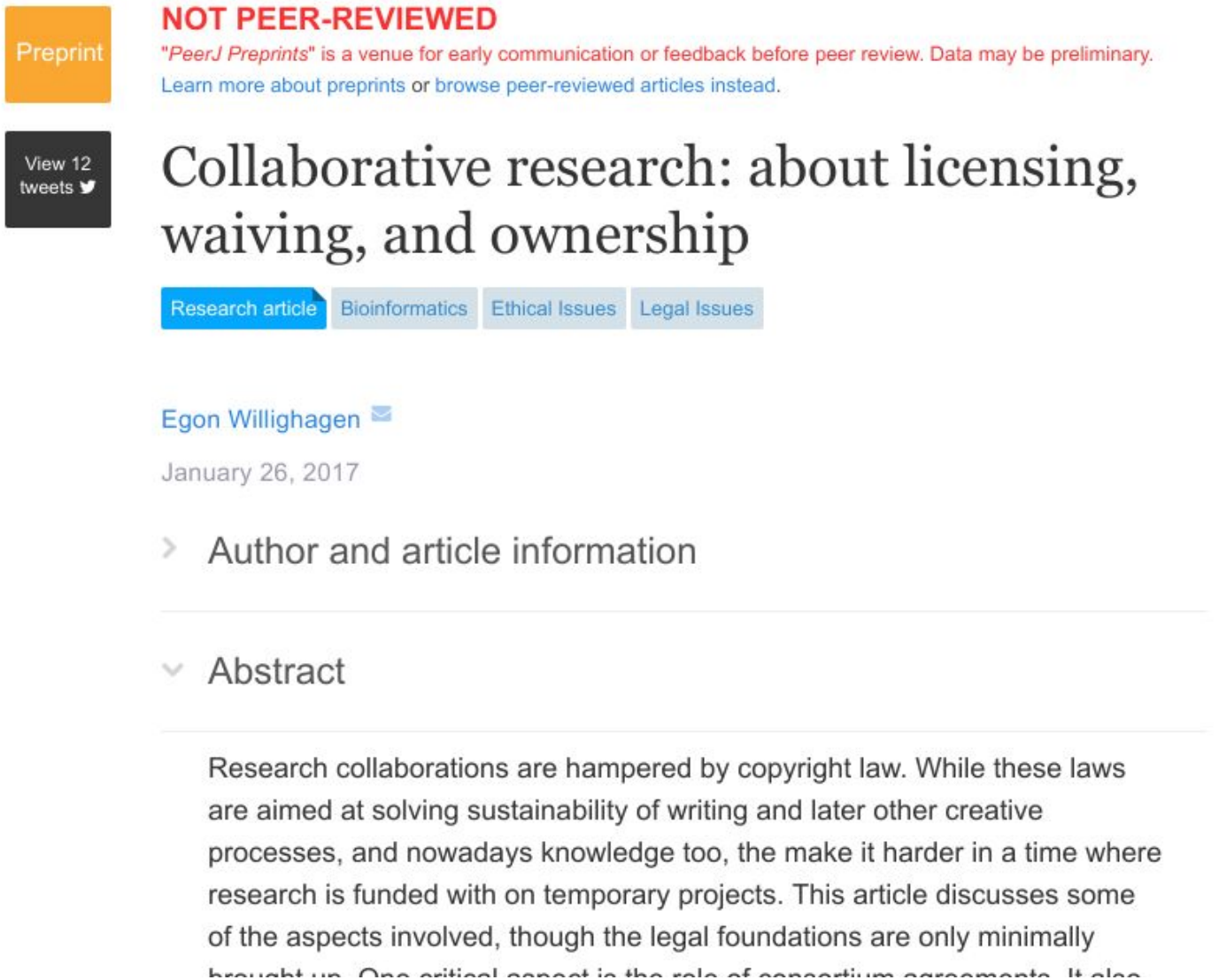
R1: clear license, provenance, community standards



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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, the 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

Gaps

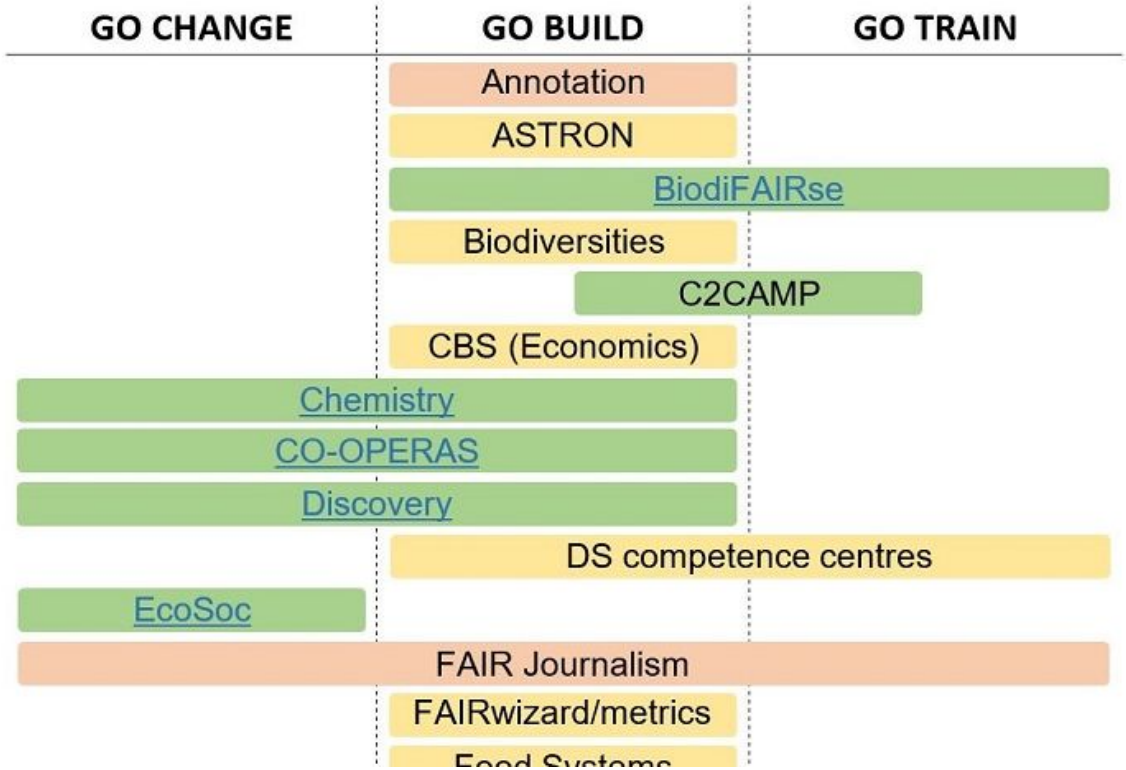
F4: specify identifiers

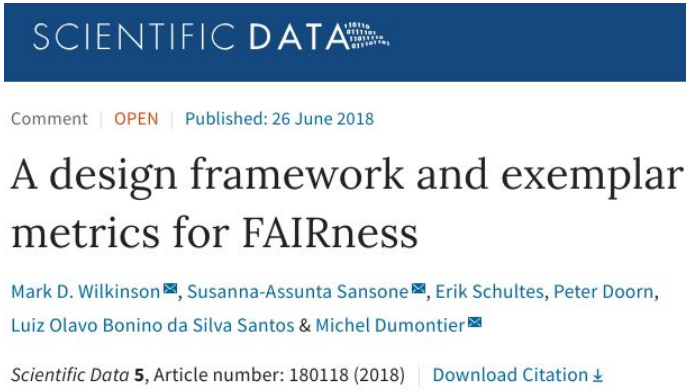
A2: metadata persistent

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

R1: clear license, provenance

GO FAIR Chemistry Implementation Network





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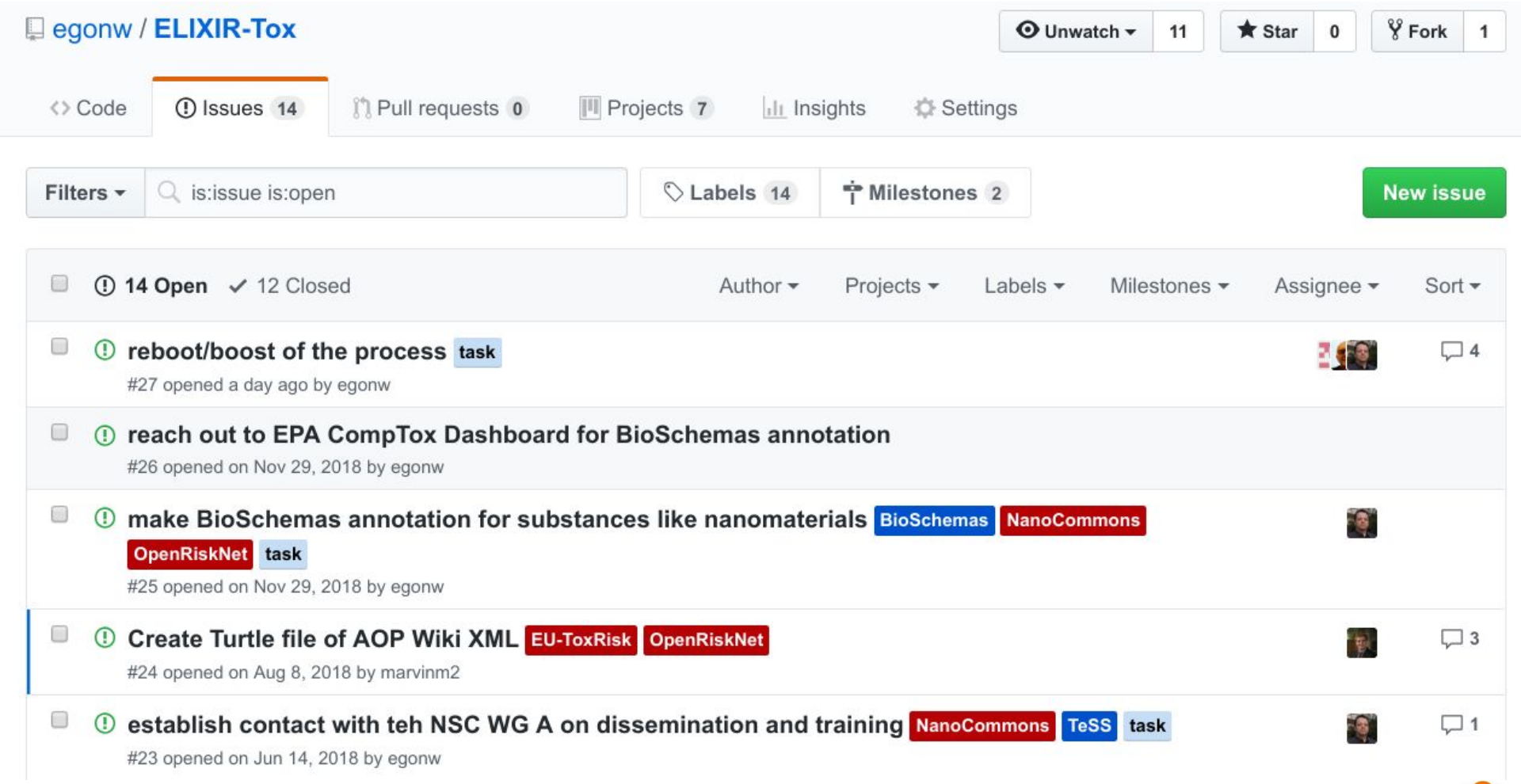
RESEARCH DATA ALLIANCE

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

ELIXIR Toxicology Community



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DTL

DUTCH TECHCENTRE FOR LIFE SCIENCES

Toxicology data management tutorials automatically collected by European training portal TeSS

Posted on 19 July 2018

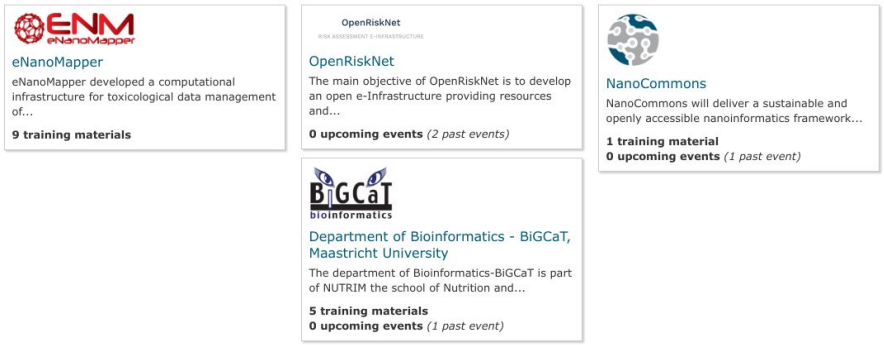
A team including Egon Willighagen from Maastricht University, Niall Beard from ELIXIR's TeSS team, and Oana Florean from Douglas Connect (coordinator of OpenRiskNet) has used BioSchemas to create a system that automatically pulls toxicology-related training materials from the eNanoMapper project into 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') t
eNanoMapper website. The scrapers run ea
team can create a scraper as long as the tar
about the tutorials," says Willighagen.



Bioschemas

Bioschemas encourages people to use sche
extensive library of simple, lightweight sche
to improve search engine visibility and inter
instance, 'Event' is a type that has properties
created schema.org extensions with life scie
sciences. This all makes it easier to discover

NanoCommons
Nano-Knowledge Community

NanoSafety Cluster

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

Using ontologies to make your research data more FAIR

Using ontologies to make your research data more FAIROverview 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,...

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