

# eNM-Ontoviewer: Interactive visualisation of SPARQL queries for eNanoMapper ontologies and data



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Within the eNanoMapper project in silico toxicology (IST) maintains the Resource Description Framework (RDF) database with nanoparticle ontologies and data. In order to simplify the combined search for data and ontologies in the eNanoMapper RDF backend, we have developed an interface for the visualisation of SPARQL queries. This poster presents the enm-ontoviewer application [1] considering two use case scenarios and links to source code and documentation.



## Use case 1: Investigate the eNanoMapper ontology

Assuming that we are interested in *toxicological endpoints* we execute the template SPARQL query to receive results either as a static *Dendogram* graph (*Figure 1*) or as an interactive *Sunburst* graph (*Figure 2*). To get all information about a subject we can use the SPARQL interface (*Figure 4*) and write another query. We are always able to refine our query or investigate directly any kind of URIs from the result (*Figure 5*).



# Figure 2: Sunburst. Result for *toxicological endpoint* search.





Figure 3: Sunburst. Interactive zoom on *dermal toxicity* endpoint.

Nanomapper Summary Classes Properties Notes Mappings Widg	ets Details Visualization	n Notes (0) Class Mappings (1) 🔗
ecotox eye irritation Immunotoxicity	Preferred Name	skin sensitization Skin sensitization is induced sensitivity to an agent that in time leads to an allergic response to
tox long term toxicity carcinogenicity	ID	http://purl.enanomapper.org/onto/ENM_0000034
<ul> <li>cytotoxicity</li> <li>dermal toxicity</li> <li>acute dermal toxicity</li> </ul>	alternative term	skin sensitisation skin sensitization
<ul> <li>repeated dose dermal toxicity</li> <li>skin irritation</li> <li>skin sensitization</li> </ul>	prefLabel	skin sensitization Skin sensitization is induced sensitivity to an agent that in time leads to an allergic response to
<ul> <li>developmental toxicity</li> <li>drug toxicity</li> <li>environmental toxicity</li> </ul>	subClassOf	that agent.
genetic toxicity     immunotoxicity     inhalation toxicity		

http://purl.enanomapper.org /onto/ENM_000018http://purl.obolibrary.org /obo/IAO_0000115"A quantitive or qualitative interpretable standardized representation of a perturbation of relevance in toxicology that is measured by a toxicological assay."http://purl.enanomapper.org /onto/ENM_000018http://www.w3.org/2000/01 /rdf-schema#label"toxicological endpoint"@en	http://purl.enanomapper.org /onto/ENM_0000018	http://www.w3.org/2000/01 /rdf-schema#subClassOf	http://www.bioassayontology.org/bao#BAO_0000179
http://purl.enanomapper.org /onto/ENM_0000018 http://www.w3.org/2000/01 /rdf-schema#label "toxicological endpoint"@en	http://purl.enanomapper.org /onto/ENM_0000018	http://purl.obolibrary.org /obo/IAO_0000115	"A quantitive or qualitative interpretable standardized representation of a perturbation of relevance in toxicology that is measured by a toxicological assay."
	http://purl.enanomapper.org /onto/ENM_0000018	http://www.w3.org/2000/01 /rdf-schema#label	"toxicological endpoint"@en

Figure 4: SPARQL interface. Select *skin sensitization* subclass endpoint from *Figure 3* for a detail query.



Figure 5: Following a link from the query result in *Figure 4* we reach the eNanoMapper ontology on BioPortal.

#### Use case 2: Investigate eNanoMapper data

**Example Queries** 

Physico-Chemical Characteristics

All ENMs have at least one chemical component

Particle Size (Distribution)

Surface charge

Assuming that we want to investigate eNanoMapper nano material data we can simply choose one of the given SPARQL examples (*Figure 6*) as a starting point. In this case we are interested in *surface charge* and search for the zeta potential and its values. We receive a table with values and resource identifiers which point us directly to the resource page of the eNanoMapper database service (*Figure 7*).

VIEWER SPARQL HELP

PREFIX chebi: <http: chebi_="" obo="" purl.obolibrary.org=""> PREFIX npo: <http: npo#="" ontology="" purl.bioontology.org=""> PREFIX obo: <http: obo="" purl.obolibrary.org=""></http:> PREFIX bao: <http: bao#="" www.bioassayontology.org=""> PREFIX sio: <http: resource="" semanticscience.org=""></http:> SELECT DISTINCT ?resource ?epLabel ?value ?unit WHERE { ?resource a chebi:59999 . OPTIONAL { ?resource obo:BFO_0000056 ?feature . ?feature a ?featureType ; obo:OBI_0000299 ?endpoint . ?endpoint sio:has-value ?value : text/html render download</http:></http:></http:>	
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PREFIX obo: <http: obo="" purl.obolibrary.org=""></http:> PREFIX bao: <http: bao#="" www.bioassayontology.org=""> PREFIX sio: <http: resource="" semanticscience.org=""></http:> SELECT DISTINCT ?resource ?epLabel ?value ?unit WHERE {     ?resource a chebi:59999 .     OPTIONAL {         ?resource obo:BFO_0000056 ?feature .         ?feature a ?featureType ;         obo:OBI_0000299 ?endpoint .         ?endpoint sio:has-value ?value :         text/html</http:>	PREFIX npo: <a href="http://purl.bioontology.org/ontology/npo#">http://purl.bioontology.org/ontology/npo#</a>
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source	epLabel	value	u
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tps://data.enanomapper.net/substance/NWKI-37e2b8ec-0e57-3ed8-9afc-93a3030ee25f	ZETA POTENTIAL	60.6	m
tps://data.enanomapper.net/substance/NWKI-ae67096a-fca6-3afc-bade-c362e3eeadc8	ZETA POTENTIAL	-15.1	m
tps://data.enanomapper.net/substance/NWKI-6a8efcf8-a19c-3fb3-b8ca-3f4e1a09fcb0	ZETA POTENTIAL	-50.4	m

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	Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	♦ Owner ♦	Info

Figure 1: Dendogram

Links

https://data.enanomapper.net/substance/NWKI-144a9226-4b93-36a9-ba2d-6b6c4903357bZETA POTENTIAL-11.0mVFigure 6: SPARQL interface. Select one of the<br/>physio-chemical characteristics examples.

Figure 7: Following a link from the query result in *Figure 6* we reach the eNanoMapper database service.

### References

- eNM Ontology Viewer https://query.enanomapper.net/enm-viewer
- eNM SPARQL interface https://sparql.enanomapper.net
- Source code https://github.com/enanomapper/enm-ontoviewer
- eNM Ontologies https://github.com/enanomapper/ontologies
- > eNM Database service https://data.enanomapper.net

[1] Denis Gebele, Micha Rautenberg, and Christoph Helma. eNanoMapper ontology viewer, January 2017. URL https://doi.org/10.5281/zenodo.259384.

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