eNanoMapper - A Database and Ontology Framework for Nanomaterials Design and Safety Assessment

ACS Meeting, Boston, USA, 18 August 2015

Presented by Barry Hardy (Douglas Connect) as Coordinator and in representation of work carried out by eNanoMapper and its partners. Any opinions or comments are made as personal statements and are not to taken as indicating any official position of any organisation.

Barry dot Hardy –(at)/- douglasconnect dot com

www.enanomapper.net

Douglas Connect
Working communities

eNM
eNanoMapper

Collaborating Partners on eNanoMapper

Douglas Connect, Switzerland (Coordinator)

Maastricht University, Netherlands

In Silico Toxicology, Switzerland

National Technical University of Athens, Greece

Ideaconsult, Bulgaria

EMBL-EBI, UK

Karolinska Instituet, Sweden

VTT, Finland

Associate Partners

eNanoMapper

Main objectives of eNanoMapper

- Modular infrastructure for data storage, sharing and searching, based on open standards and semantic web technologies, minimum information standards and established security solutions
- Development of ontologies for the categorisation and characterisation of Engineered Nanomaterials (ENMs) in collaboration with other projects
- Creation of new computational models in nanomaterials safety through the implementation of interfaces for toxicity modelling and prediction algorithms which may process all data made available through eNanoMapper (e.g. using algorithms available from the OpenTox project or statistical/data mining software)

eNM
eNanoMapper

Main objectives of eNanoMapper

- **Meta analysis of nano-bio interactions supporting "safe-by-design" ENMs development by pursuing a Linked Data approach which integrates data and metadata originating from diverse sources within nanoscience, chemistry, biology and toxicology**
- **Creation of tools for the exchange, quality assurance and reporting of research protocols and data for regulatory purposes**
- **Creation of a community framework for interdisciplinary collaboration**

eNanoMapper

OpenTox and Open Components and Standards

<-New API addition from ToxBank

Investigation (Study, Assay)
GET
POST
PUT
DELETE

Authorisation & Authentication
GET
POST
PUT
DELETE

Dataset
GET
POST
PUT
DELETE

Feature
GET
POST
PUT
DELETE

Compound
GET
POST
PUT
DELETE

AppDomain
GET
POST
PUT
DELETE

Model
GET
POST
PUT
DELETE

Algorithm
GET
POST
PUT
DELETE

Report
GET
POST
PUT
DELETE

Validation
GET
POST
PUT
DELETE

Ontology
GET
POST
PUT
DELETE

OpenTox

www.opentox.org/dev/apis/api-1.2

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A Toxicology Ontology Roadmap

- See perspectives and roadmap published in A Toxicology Ontology Roadmap ALTEX 29(2), 129- 137 and Toxicology Ontology Perspectives 139 - 156 (2012)
- Available online in Open Access mode from www.altex.ch
- Barry Hardy (Douglas Connect and OpenTox), Gordana Apic (Cambridge Cell Networks), Philip Carthew (Unilever), Dominic Clark (EMBL-EBI), David Cook (AstraZeneca), Ian Dix (AstraZeneca & Pistoia Alliance), Sylvia Escher (Fraunhofer Institute for Toxicology & Experimental Medicine), Janna Hastings (EMBL-EBI), David J. Heard (Novartis), Nina Jeliazkova (Ideaconsult), Philip Judson (Lhasa Ltd.), Sherri Matis-Mitchell (AstraZeneca), Dragana Mitic (Cambridge Cell Networks), Glenn Myatt (Leadscope), Imran Shah (US EPA), Ola Spjuth (University of Uppsala), Olga Tcheremenskaia (Istituto Superiore di Sanità), Luca Toldo (Merck KGaA), David Watson (Lhasa Ltd.), Andrew White (Unilever), Chihae Yang (Altamira)

*Based on Proceedings from the **Toxicology Ontology Roadmap Workshop***

EMBL-EBI Industry Programme Workshop

16 -17th November 2010, Hinxton, UK

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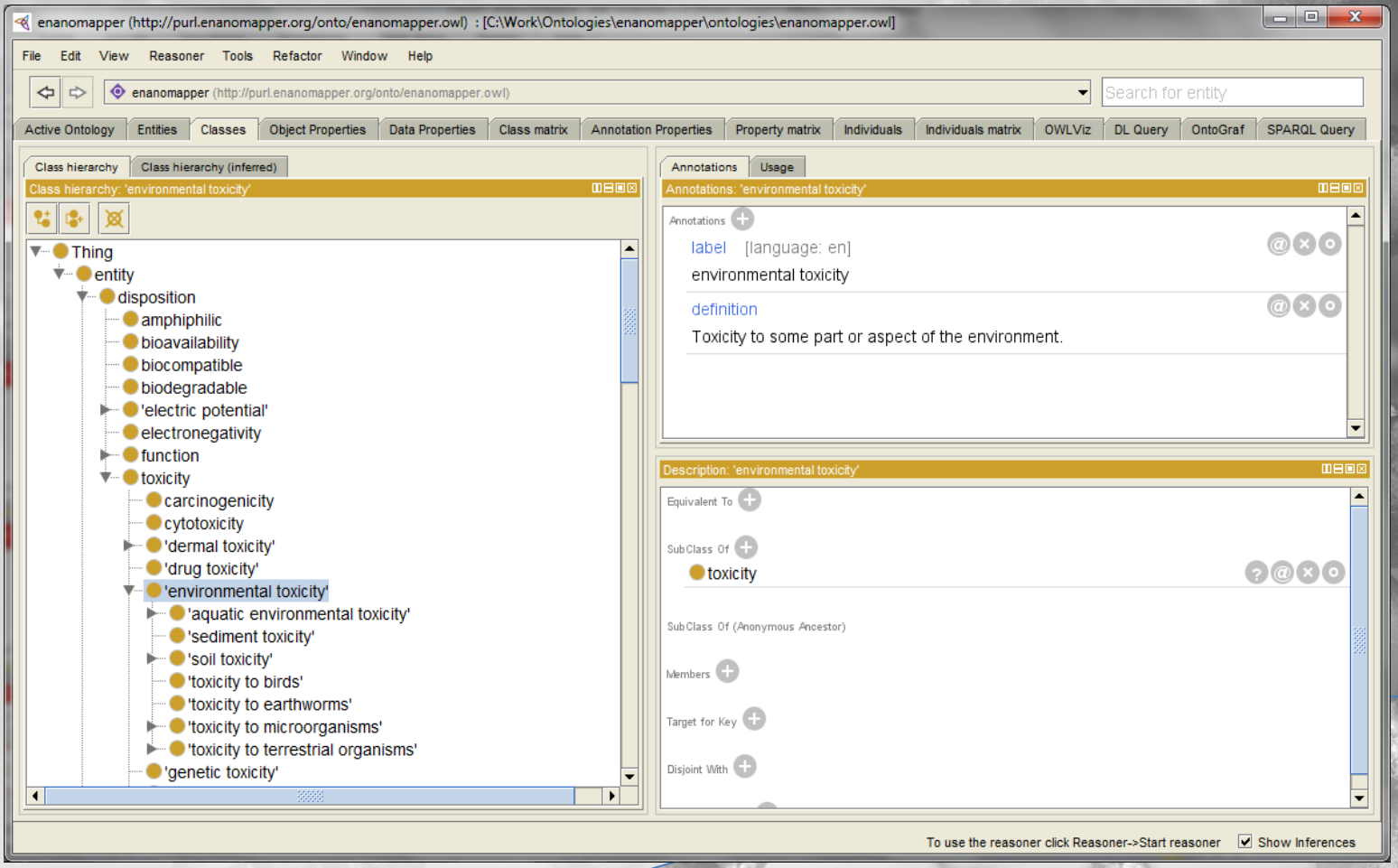
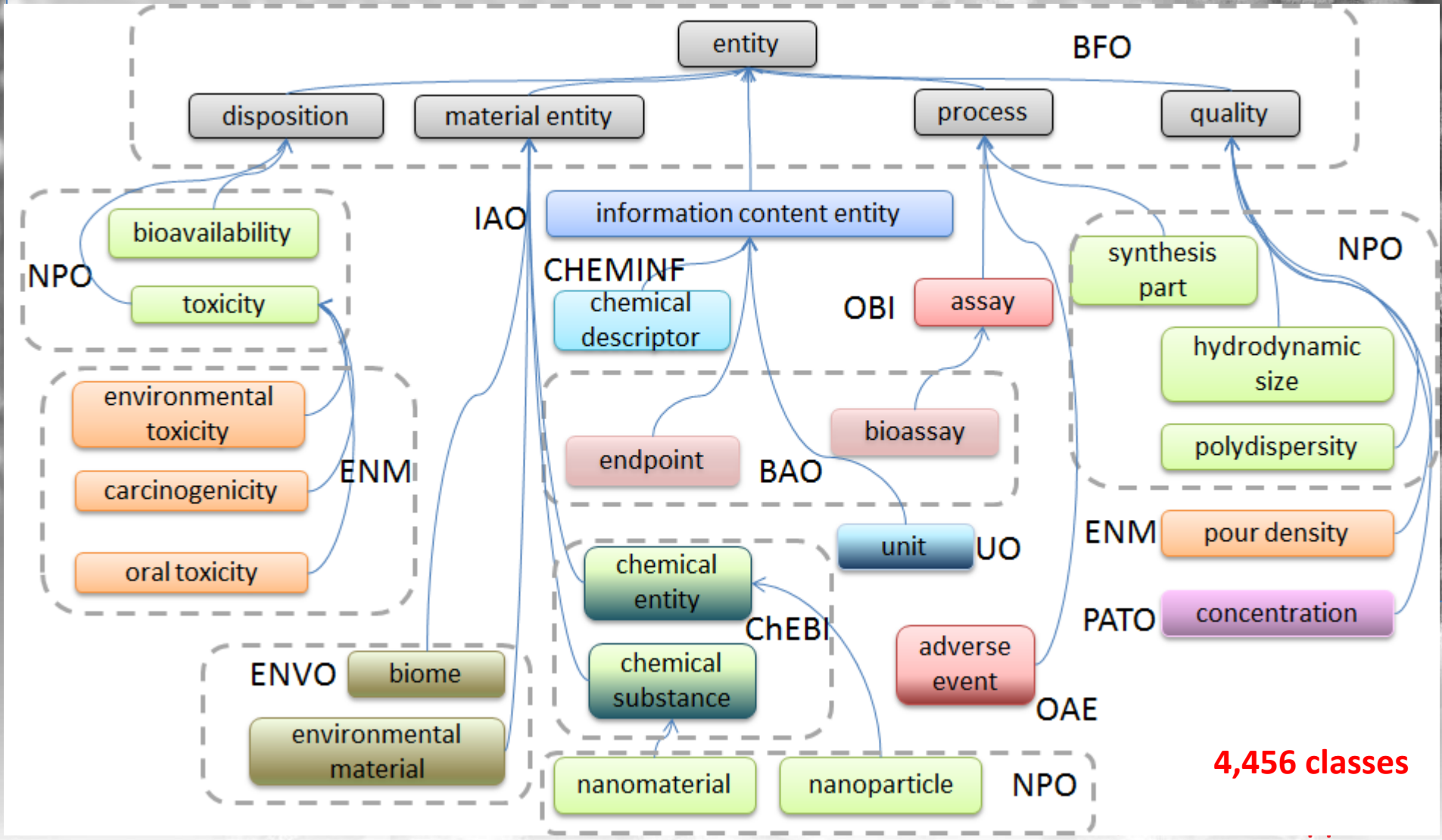
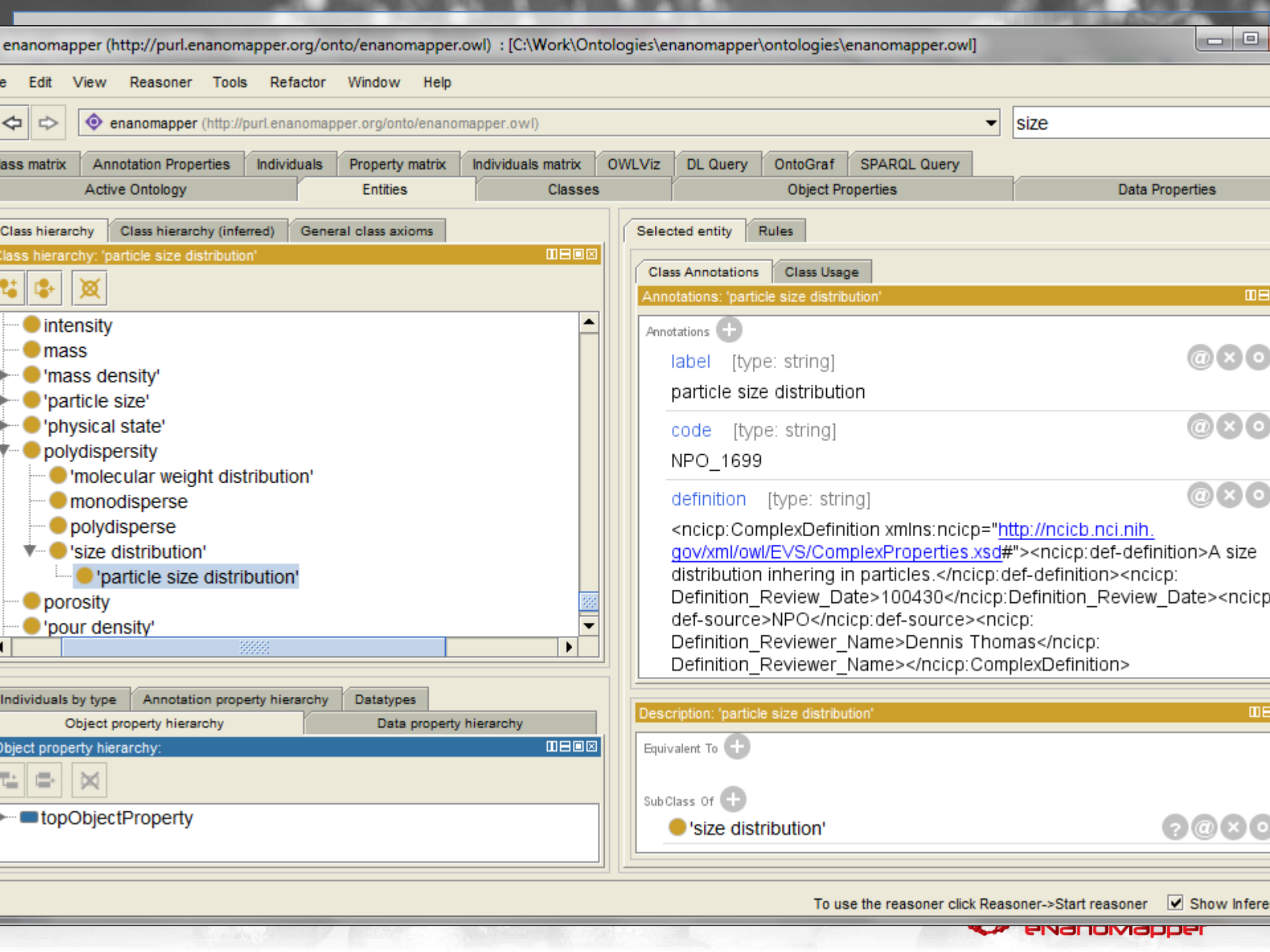
Prototype eNanoMapper ontology



Ontology assembled from multiple sources




enanomapper (http://purl.enanomapper.org/onto/enanomapper.owl) : [C:\Work\Ontologies\enanomapper\ontologies\enanomapper.owl]
Edit View Reasoner Tools Refactor Window Help
enanomapper (http://purl.enanomapper.org/onto/enanomapper.owl)
size
ass matrix Annotation Properties Individuals Property matrix Individuals matrix OWLViz DL Query OntoGraf SPARQL Query
Active Ontology Entities Classes Object Properties Data Properties
Class hierarchy Class hierarchy (inferred) General class axioms
lass hierarchy: 'particle size distribution'
intensity
mass
'mass density'
'particle size'
'physical state'
polydispersity
'molecular weight distribution'
monodisperse
polydisperse
'size distribution'
'particle size distribution'
porosity
'pour density'
Individuals by type Annotation property hierarchy Datatypes
Object property hierarchy Data property hierarchy
bject property hierarchy:
topObjectProperty
Selected entity Rules
Class Annotations Class Usage
Annotations: 'particle size distribution'
Annotations
label [type: string]
particle size distribution
code [type: string]
NPO_1699
definition [type: string]
<ncicp:ComplexDefinition xmlns:ncicp="http://ncicb.nci.nih.gov/xml/owl/EVS/ComplexProperties.xsd#"><ncicp:def-definition>A size distribution inhering in particles.</ncicp:def-definition><ncicp:Definition_Review_Date>100430</ncicp:Definition_Review_Date><ncicp:def-source>NPO</ncicp:def-source><ncicp:Definition_Reviewer_Name>Dennis Thomas</ncicp:Definition_Reviewer_Name></ncicp:ComplexDefinition>
Description: 'particle size distribution'
Equivalent To
SubClass Of
'size distribution'
To use the reasoner click Reasoner->Start reasoner
Show Infere

eNanoMapper Ontology in BioPortal

eNanoMapper

Summary Classes Properties Notes Mappings Widgets

Details

ACRONYM	ENM
VISIBILITY	Public
BIOPORTAL PURL	http://purl.bioontology.org/ontology/ENM
DESCRIPTION	The eNanoMapper ontology covers the full scope of terminology needed to support research into nanomaterial safety. It builds on multiple pre-existing external ontologies such as the NanoParticle Ontology.
STATUS	Alpha
FORMAT	OWL
CONTACT	Egon Willighagen, egon.willighagen@gmail.com Janna Hastings, hastings@ebi.ac.uk
HOME PAGE	https://github.com/enanomapper/ontologies
PUBLICATIONS PAGE	
DOCUMENTATION PAGE	
CATEGORIES	Health
GROUPS	

Metrics

NUMBER OF CLASSES:	4555
NUMBER OF INDIVIDUALS:	177
NUMBER OF PROPERTIES:	652
MAXIMUM DEPTH:	10
MAXIMUM NUMBER OF CHILDREN:	91
AVERAGE NUMBER OF CHILDREN:	4
CLASSES WITH A SINGLE CHILD:	354
CLASSES WITH MORE THAN 25 CHILDREN:	34
CLASSES WITH NO DEFINITION:	1089

Visits

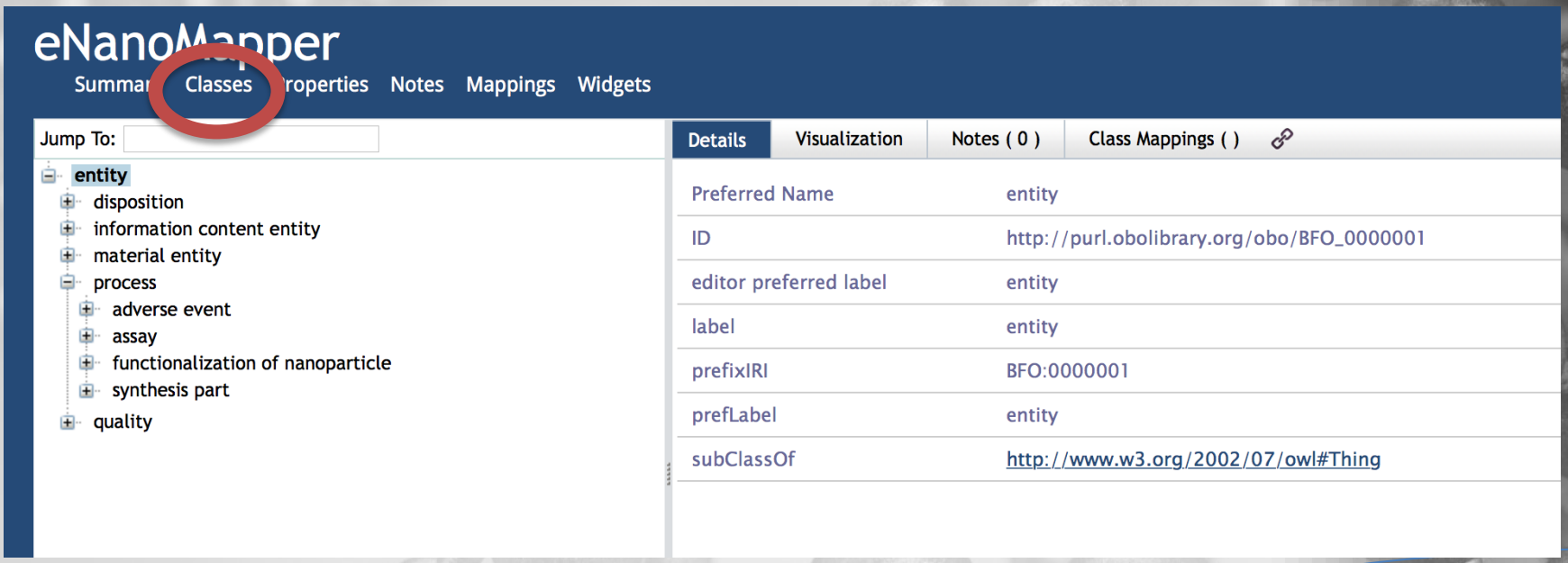
Download as CSV

90
80
70

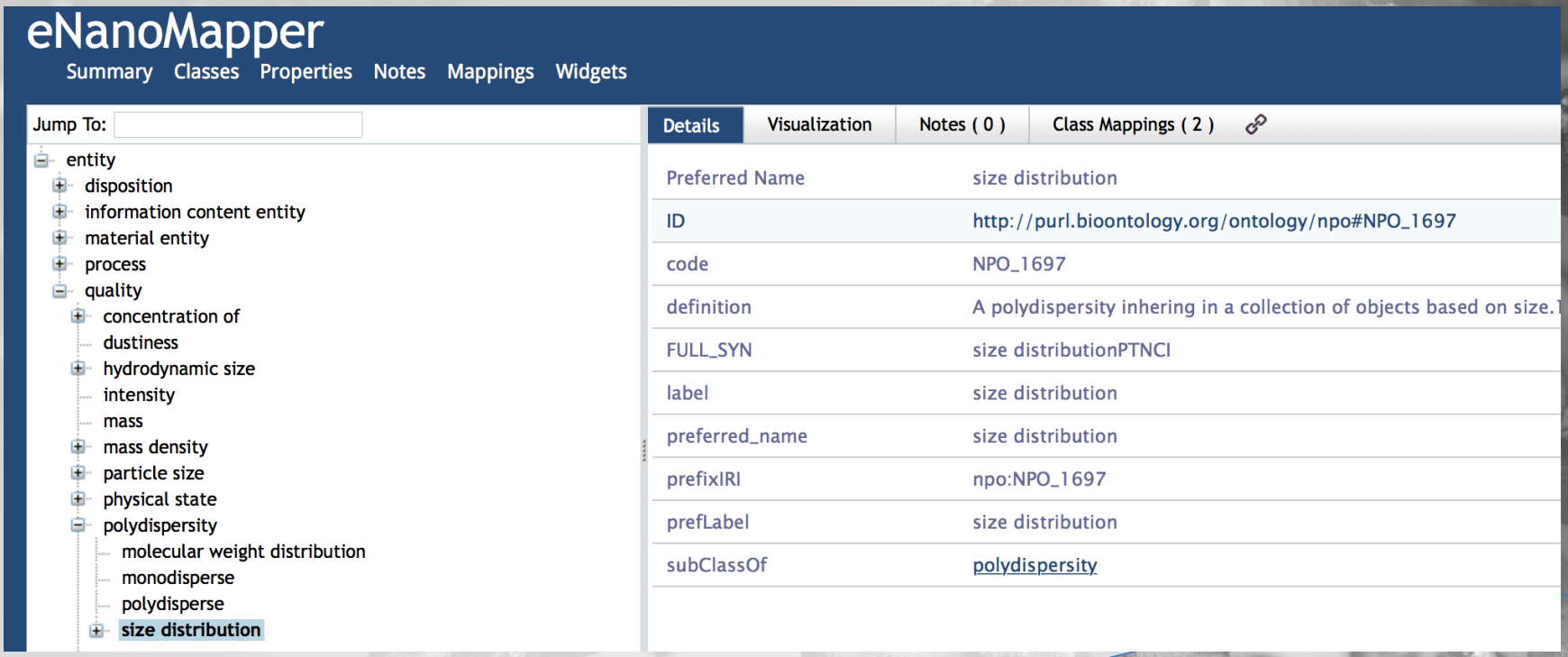
bioportal.bioontology.org/ontologies/ENM

ENM eNanoMapper

Browse classes

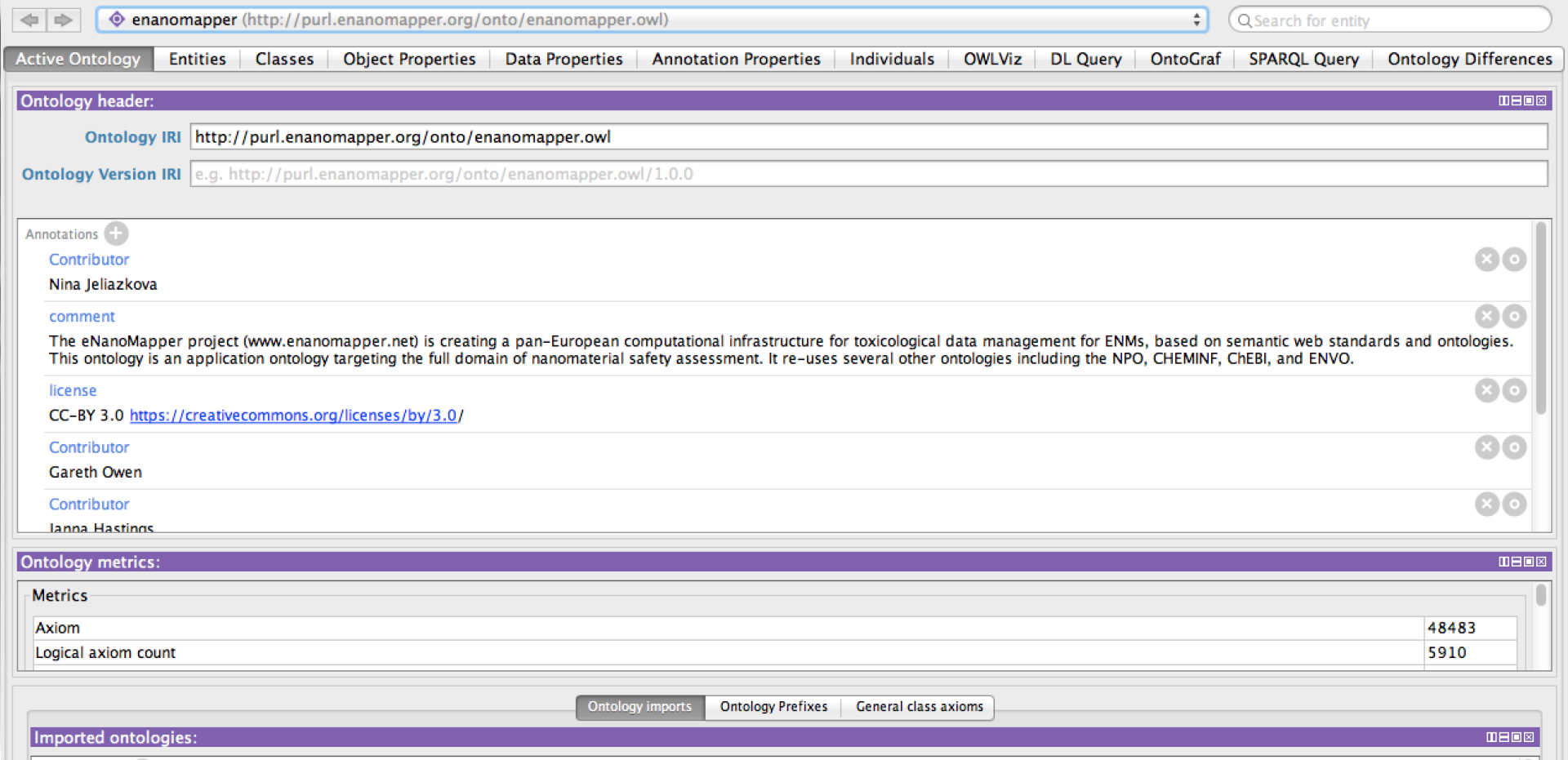


View metadata (synonyms, ID)

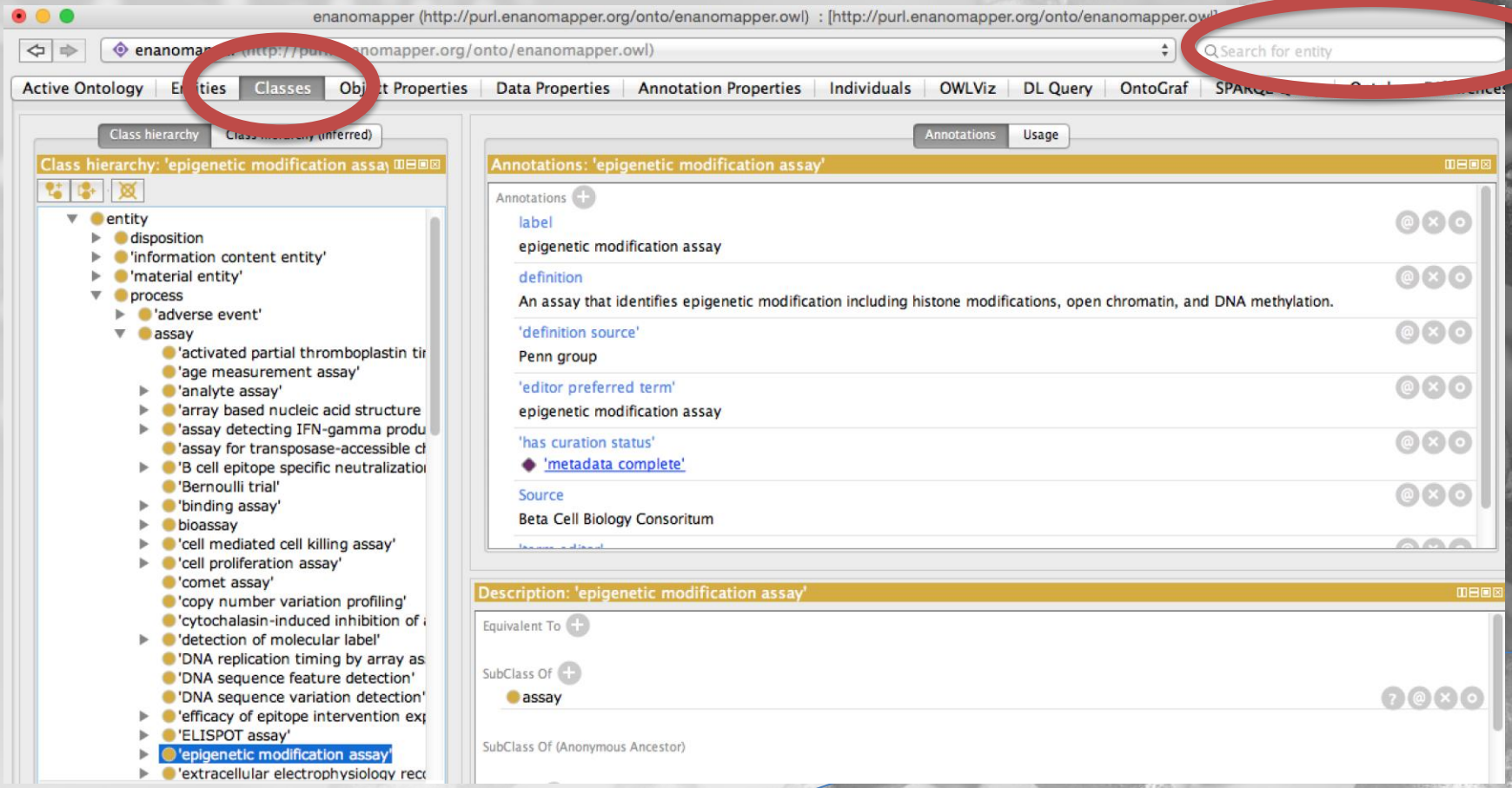


eNanoMapper Ontology in Protegé

Open in Protegé purl.enanomapper.org/onto/enanomapper.owl

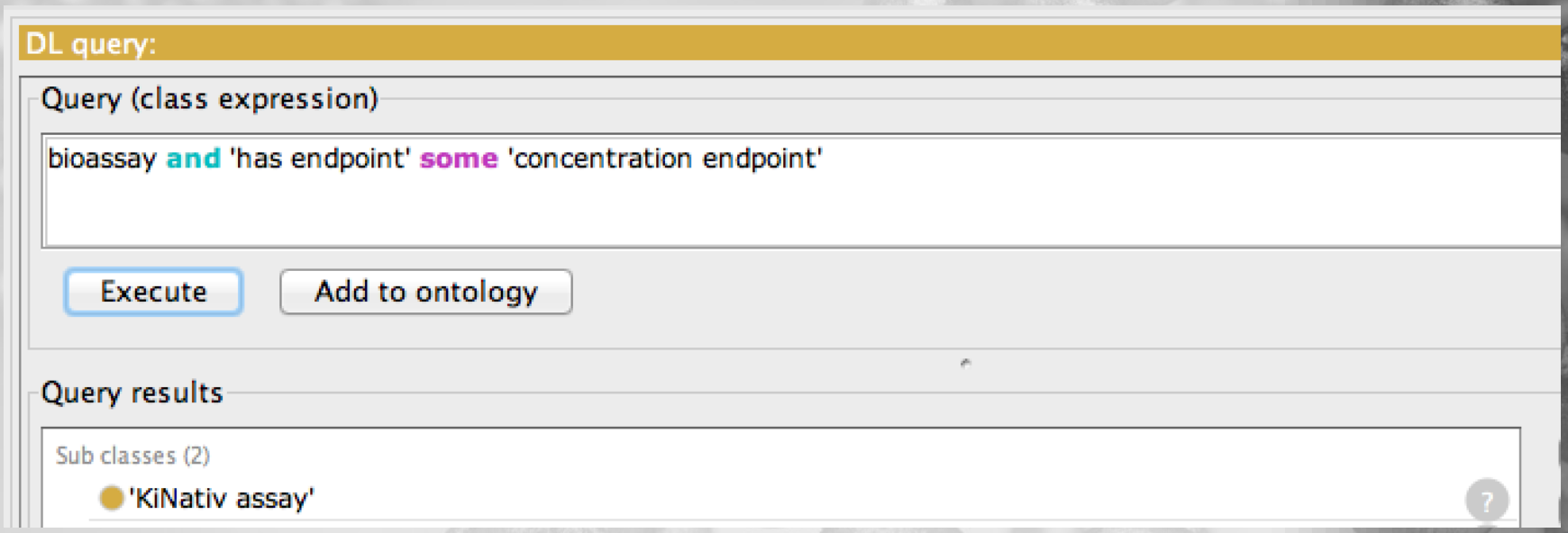


Browse, Search

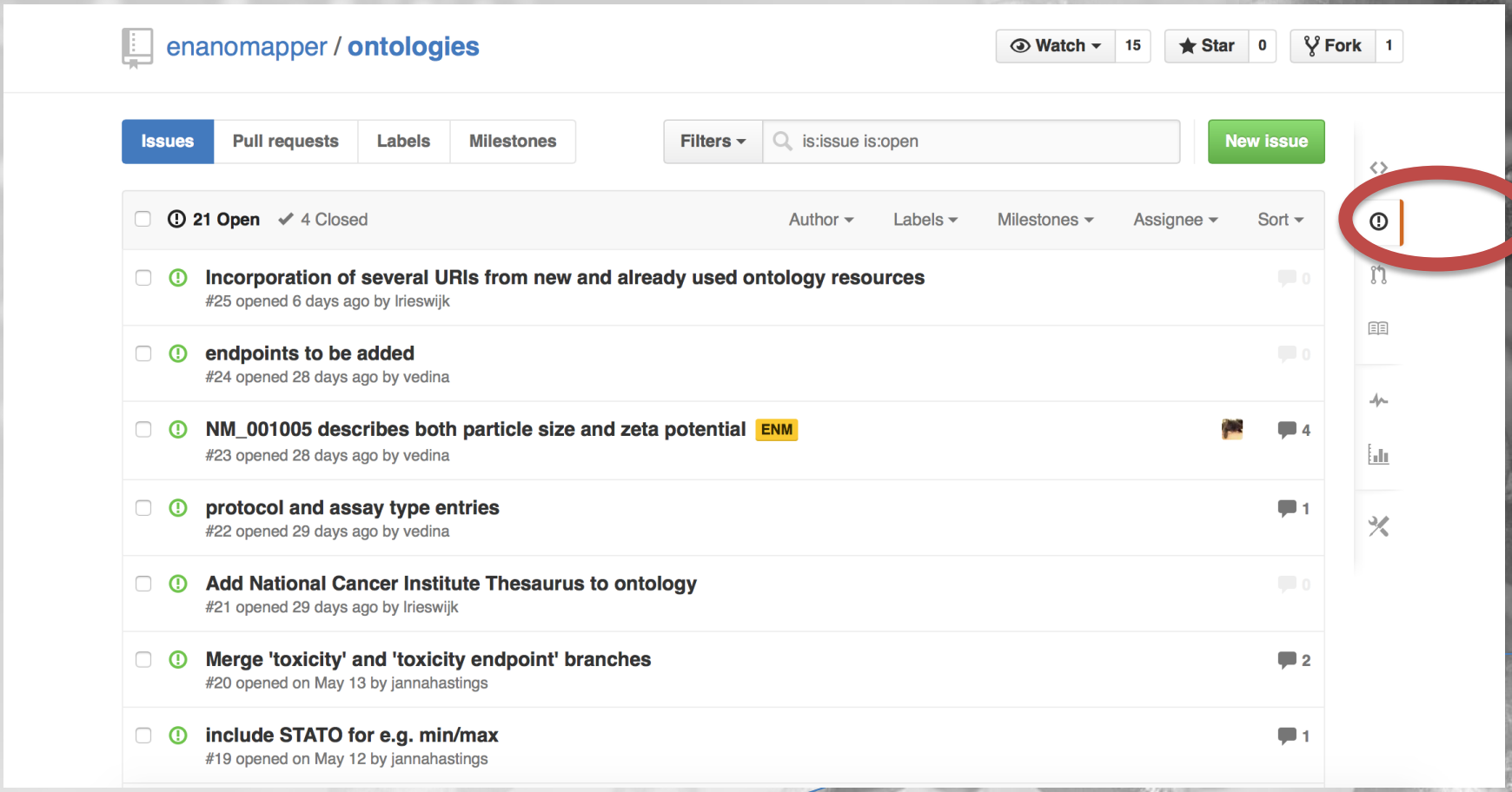


eNanoMapper

Logic-based querying



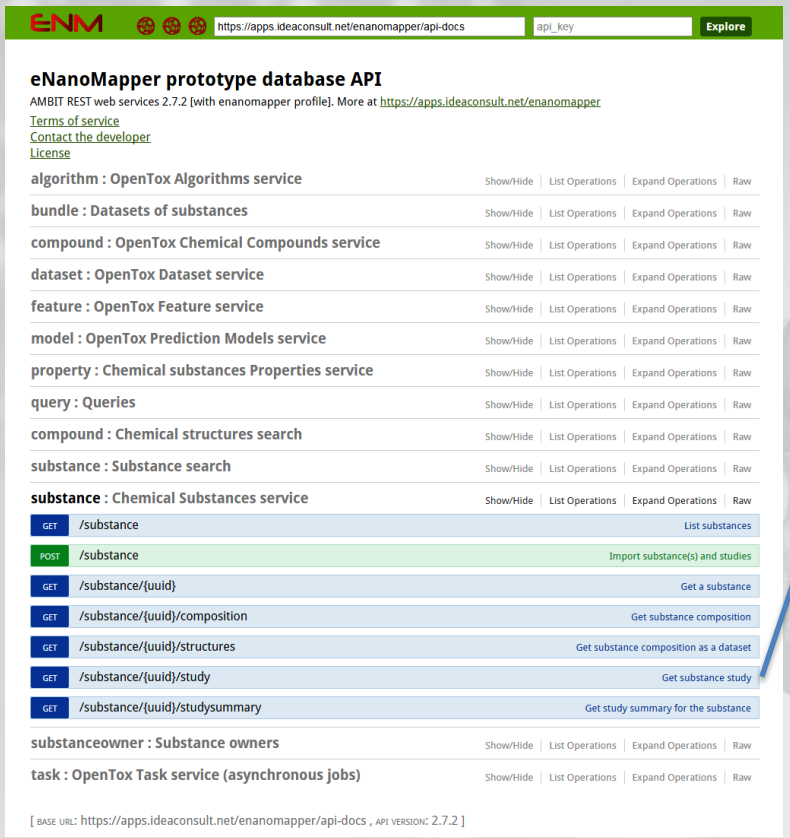
GitHub enanomapper ontologies



ENM eNanoMapper

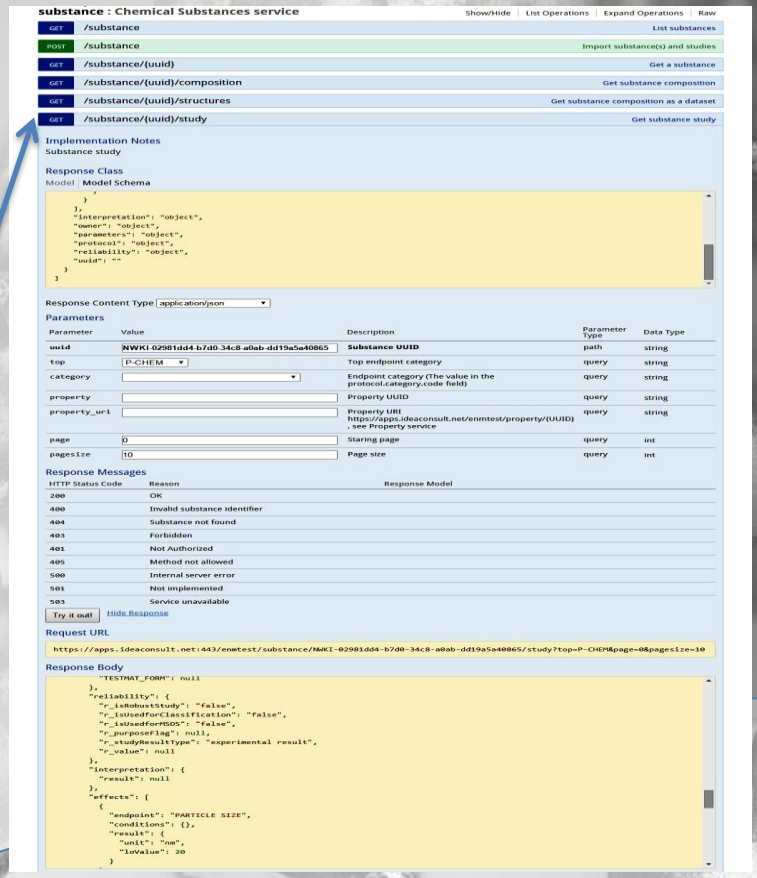
REST Application Programming Interface

API documentation (Swagger-UI)

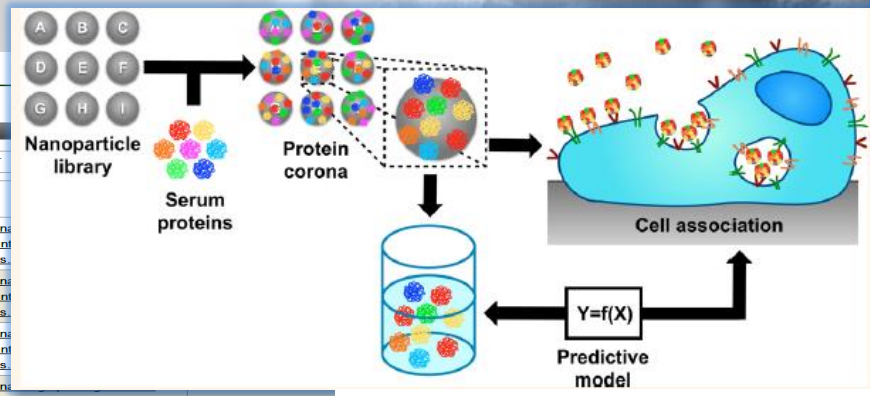


http://enanomapper.github.io/API/

Interactive API queries



Prototype database (NM components)



Protein Corona Data set
DOI:10.1021/nn406018q

eNM eNanoMapper

Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

Search substances by identifiers

Showing from 1 to 100 in pages of 100 substances Previous Next

DDT

	Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID		
- 11 -	G15.DDT@BDHDA	FCSV-2a853f39-4...	nanoparticle	G15.DDT@BDHDA	FCSV-2a853f39-4...	Protein Corona the Cellular Int Nanoparticles	
- 12 -	G15.DDT@CTAB	FCSV-d1731b11-2...	nanoparticle	G15.DDT@CTAB	FCSV-d1731b11-2...	Protein Corona the Cellular Int Nanoparticles	
- 13 -	G15.DDT@DOTAP	FCSV-3b96ad7a-b...	nanoparticle	G15.DDT@DOTAP	FCSV-3b96ad7a-b...	Protein Corona the Cellular Int Nanoparticles	
- 14 -	G15.DDT@ODA	FCSV-fb5e6048-8...	nanoparticle	G15.DDT@ODA	FCSV-fb5e6048-8...	Protein Corona the Cellular Interaction of Gold and Silver Nanoparticles.csv	

Composition name:
Composition UUID: FCSV-fb5e6048-8ee1-351d-915b-d1669681357e
Purity of IUC Substance:

Type	Name	EC No.	CAS No.	Typical concentration	Concentration ranges			Structure
Coating	Dodecane-1-Thiol,Wnahizmdsqcwrp-Uhfffaoysa-N,Inchi=1s/C12h26s/C1-2-3-4-5-6-7-8-9-10-11-12-13/H13h,2-12h2,1h3,1-Dodecanethiol			0 % (w/w)	0 % (w/w)	0 % (w/w)	Also contained in...	
Coating	Octadecan-1-Amine,Reyjpsvuyrzge-Uhfffaoysa-N,Inchi=1s/C18h39n/C1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/H2-19h2,1h3,Stearylamine,1-Octadecanamine,Octadecylamine			0 % (w/w)	0 % (w/w)	0 % (w/w)	Also contained in...	
Core	[Au]			0 % (w/w)	0 % (w/w)	0 % (w/w)	Also contained in...	Au

Search:

Coating

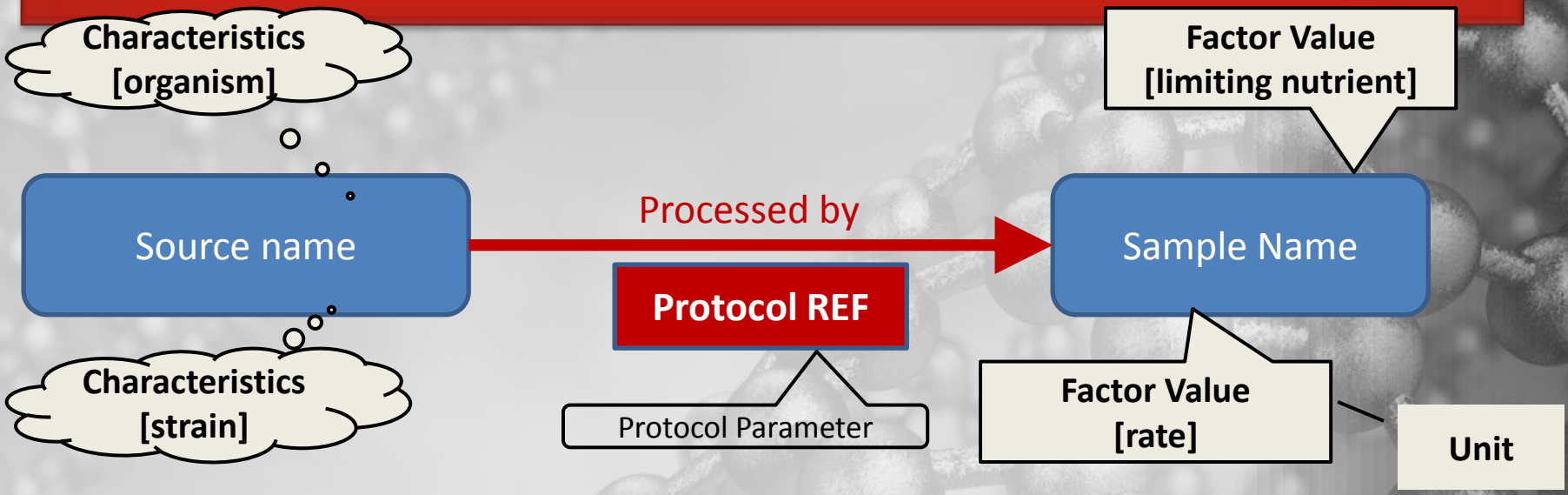
Coating

Core

- 15 -	G15.DDT@SA	FCSV-cd7105f2-f...	nanoparticle	G15.DDT@SA	FCSV-cd7105f2-f...	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Anionic
- 16 -	G15.DDT@SDS	FCSV-9505d90b-f...	nanoparticle	G15.DDT@SDS	FCSV-9505d90b-f...	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Anionic
- 68 -	G30.DDT@BDHDA	FCSV-50aee86c-a...	nanoparticle	G30.DDT@BDHDA	FCSV-50aee86c-a...	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic
- 69 -	G30.DDT@CTAB	FCSV-c4e9df58-f...	nanoparticle	G30.DDT@CTAB	FCSV-c4e9df58-f...	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic

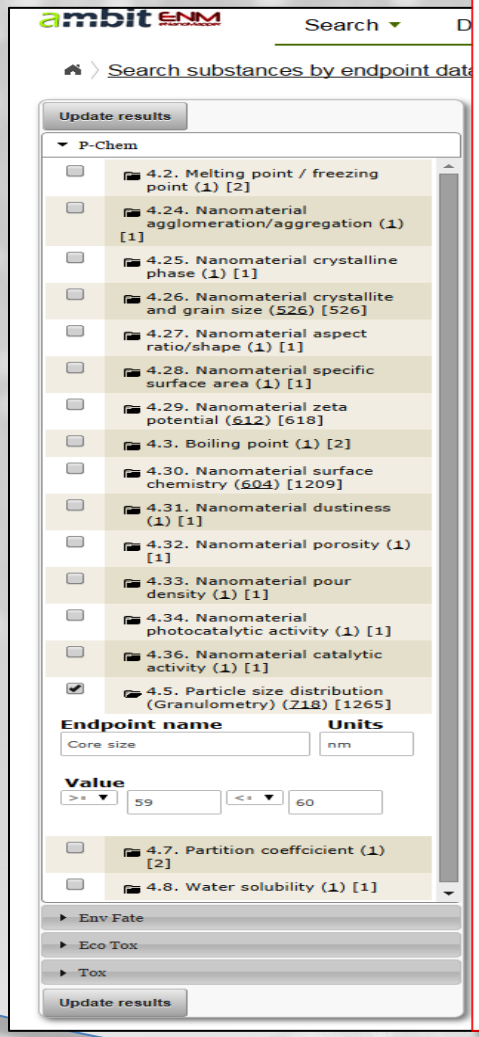
data.enanomapper.net

The Experimental graph



Source Name	Characteristics [organism]	Characteristics [strain]	Protocol REF	Sample Name	Factor Value [limiting nutrient]	Factor Value [rate]	Unit
culture1	Saccharomyces cerevisiae	FY1679	growth protocol	C-0.07-aliquot1	carbon	0.07	l/hour
culture4	Saccharomyces cerevisiae	FY1679	growth protocol	N-0.07-aliquot1	nitrogen	0.07	l/hour
culture5	Saccharomyces cerevisiae	FY1679	growth protocol	N-0.1-aliquot1	nitrogen	0.1	l/hour

ENM data in Ambit



IUC Substance | Composition | P-Chem (6) | Tox (5)

G60.AUT

4.5 Particle size distribution (Granulometry) (2)

Type of method	Test Material Form	Pass num	Endpoint	Value	Medium	Guideline	Study y..	O..	Instruments	UUI
DLS	-	-	Z-Average Hydrodynamic Diameter	mean 81.01 nm	Human serum (Si	doi: 10.1021/nn4060	2014	-	ZetaSizer Nano ZS (Malv	PR..
		-	Z-Average Hydrodynamic Diameter	mean 108.27 nm						
		-	Volume Mean Hydrodynamic Diameter	= 68.59 nm	Human serum (Si					
		-	Volume Mean Hydrodynamic Diameter	= 244.57 nm						
		-	Number Mean Hydrodynamic Diameter	= 87.28 nm	Human serum (Si					
		-	Number Mean Hydrodynamic Diameter	= 88.72 nm						
		-	Intensity Mean Hydrodynamic Diameter	= 87.28 nm	Human serum (Si					
		-	Intensity Mean Hydrodynamic Diameter	= 121.04 nm						
TEM	-	-	Core size	mean 59.3 nm	-	doi: 10.1021/nn4060	2014	-	Tecnai 20 (FEI) microsco	PR..
		-	Density	= 19.1 g/cm^3	-					
		-	MW	= 197 g/mol	-					
		-	Mol/NP	= 0	-					
		-	SA/NP	= 0 cm^2/NP	-					

Showing 2 study(s) (1 to 2) Previous Next

4.26 Nanomaterial crystallite and grain size (1)

Method type	Test Material Form	Endpoint	Result	Medium	Guideline	Study y..	O..	UUID
DLS	-	Polydispersity index	mean 0.099 nm	Human serum (Sigma #H452	doi: 10.1021/nn406018q	2014	-	PRCR-4294c373-c2d8-..
		Polydispersity index	mean 0.086 nm					

Showing 1 study(s) (1 to 1) Previous Next

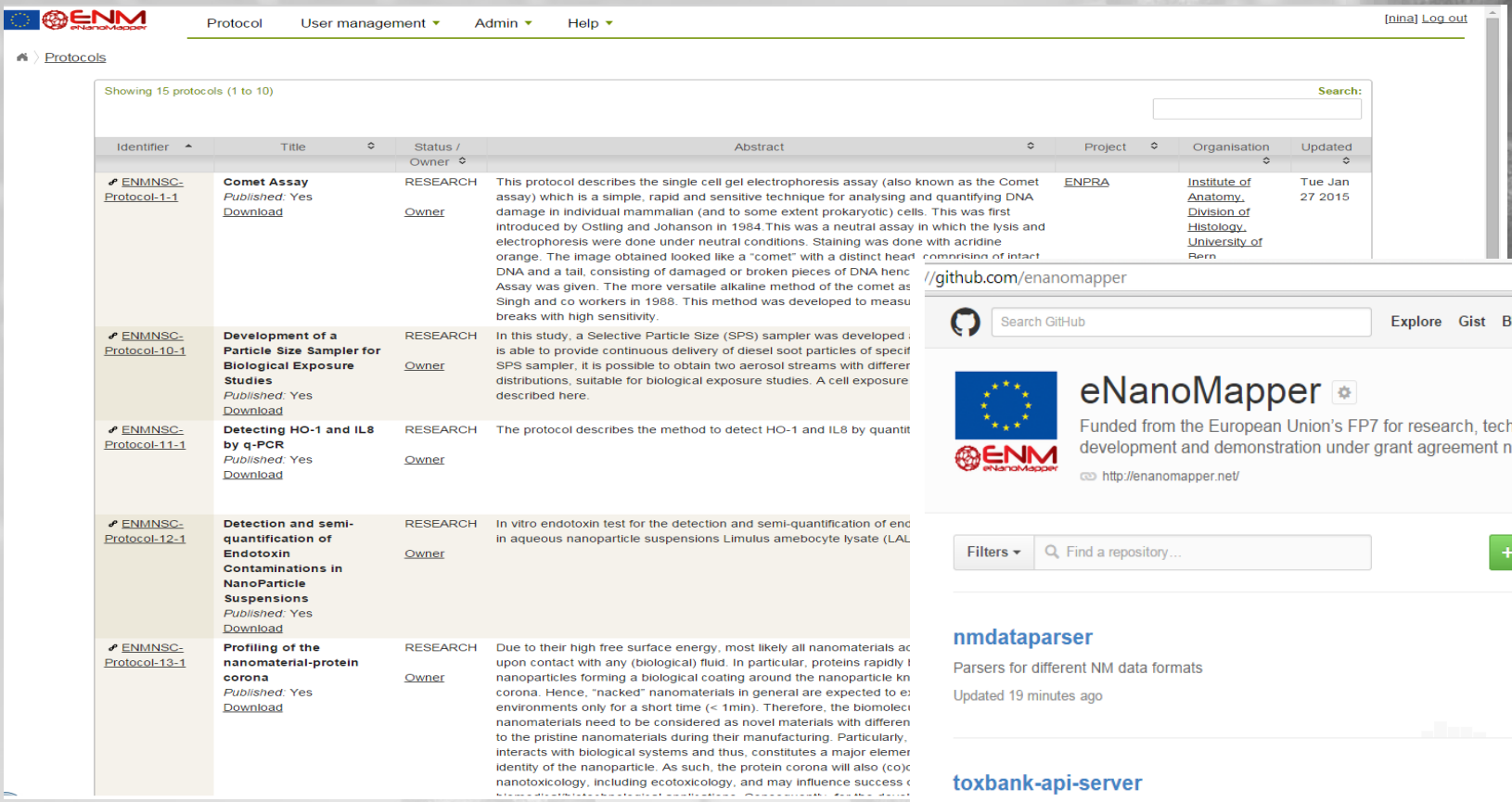
4.29 Nanomaterial zeta potential (1)

Type of method	Endpoint	Test Material Form	Result	Rem	pH	Medium	Guideline	Study y..	O..	UUID
DLS	ZETA POTENTIAL	-	mean 19.11 mv	-	-	Human serum (Sigma #H4	doi: 10.1021/nn406018q	2014	-	PRCR-a92ea051-d709..
	ZETA POTENTIAL		mean -11.47 mv	-	-					

Showing 1 study(s) (1 to 1) Previous Next

eNanoMapper

Protocol service



Analysis & Modelling

- OpenTox API Adjustments and Extensions (documented through swagger, http://enanomapper.ntua.gr:8080/jaqpot/swagger/)
  - Introduction of PMML support for descriptor definition and model reporting (allows seamless cross-platform transfer of the models produced)
  - Data preprocessing procedures (scaling, normalization, missing value handling) and calculation of domain of applicability through one algorithm call to increase efficiency and avoid creation of intermediate data sets
- Descriptor Calculation Algorithms and Methods
  - Utilization of MOPAC OpenTox service for developing Quantum mechanical descriptors for metal oxides
  - Development of web tool for image descriptor calculations. Source code: https://github.com/enanomapper/imageAnalysis , First prototype: http://enanomapper.ntua.gr:8880/imageAnalysis/
  - Gene Ontology (GO) descriptors (clustering of proteomics data based on Gene Ontology information, implemented in R language)
  - Extended the Java-based Chemistry Development Kit (CDK) with nanomaterial descriptors

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Analysis & Modelling

- NanoQSAR algorithm and modelling services
  - Extensions and updates of algorithm and modelling services to be compatible with API extensions and support of eNanoMapper Database (Access to algorithm and modelling services through swagger, http://enanomapper.ntua.gr:8080/jaqpot/swagger/#!/aa/login)
  - Integration of third party services: R language (OpenCPU), Python, WEKA
  - Development of R tool for the creation of optimal QSAR models (RRegrs, https://github.com/enanomapper/RRegrs/tree/master/RRegrs)
  - Creation of QSAR models for predicting cell association of gold nanoparticles using corona information
  - Ingenuity Pathway Analysis (IPA): Variable selection using GO descriptors/RRegrs and PLS/VIP methods on corona data. Enrichment Analysis using Ingenuity Pathway Analysis (IPA) software.

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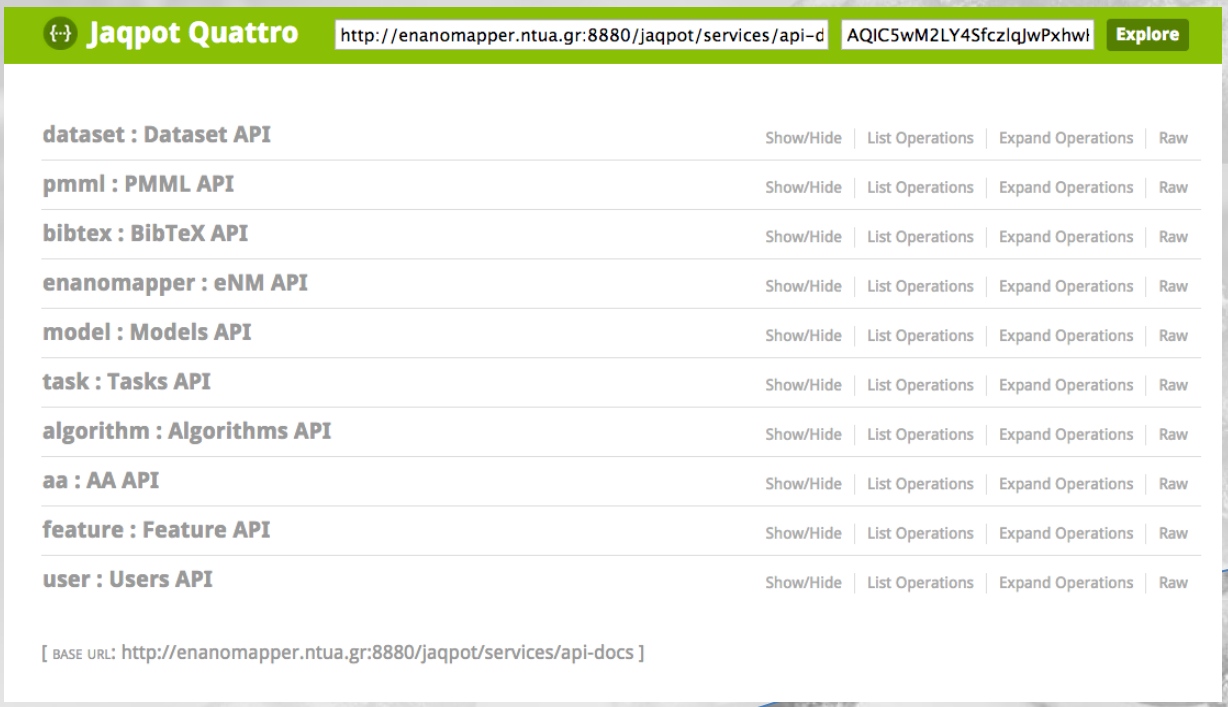
Modelling Infrastructure

- Web service standards for modelling: http://enanomapper.ntua.gr:8080/jaqpot/swagger/



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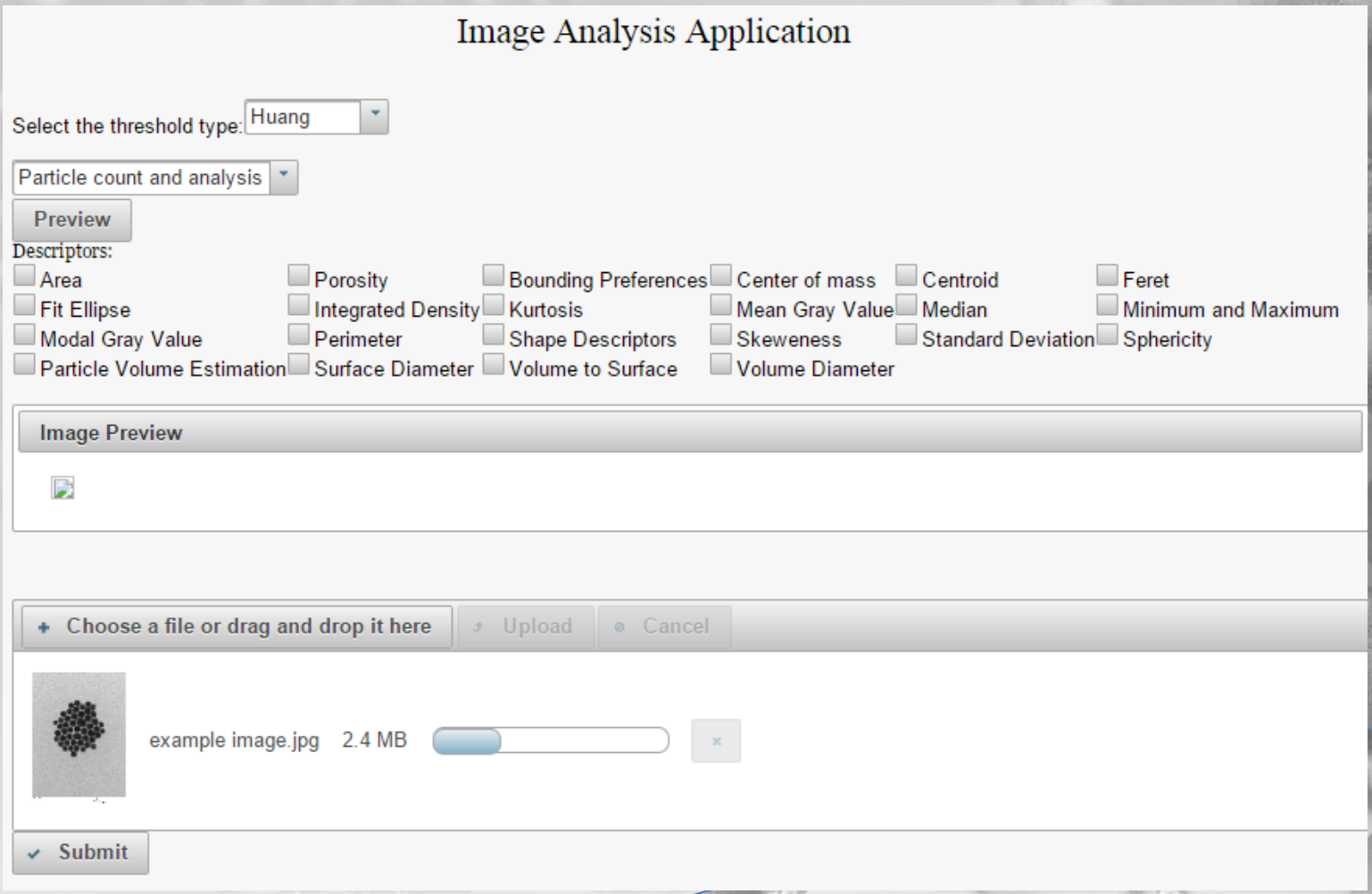
eNanoMapper

Modelling Infrastructure



Development of NanoQSAR models for predicting cell association using corona information (OpenTox models)

POST /algorithm/{id} — Creates Model

Implementation Notes

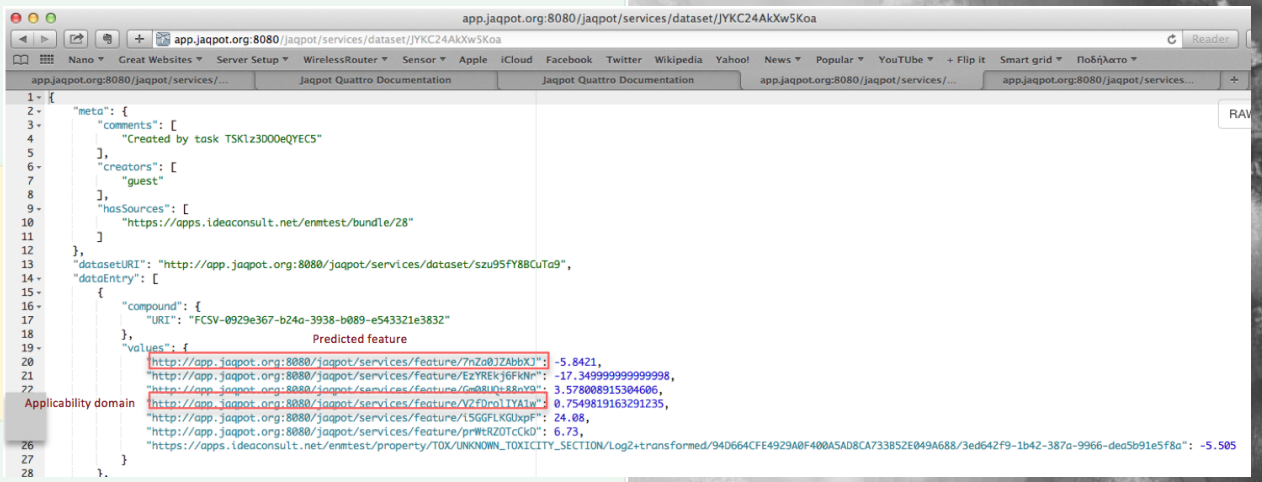
Applies Dataset and Parameters on Algorithm and creates Model.

Response Class (Status)

Model | Model Schema

```
{
  "resultUri": "",
  "result": "",
  "percentageCompleted": 0,
  "errorReport": {
    "code": "",
    "actor": "",
    "message": "",
    "details": "",
    "httpStatus": 0,
```

Response Content Type application/json



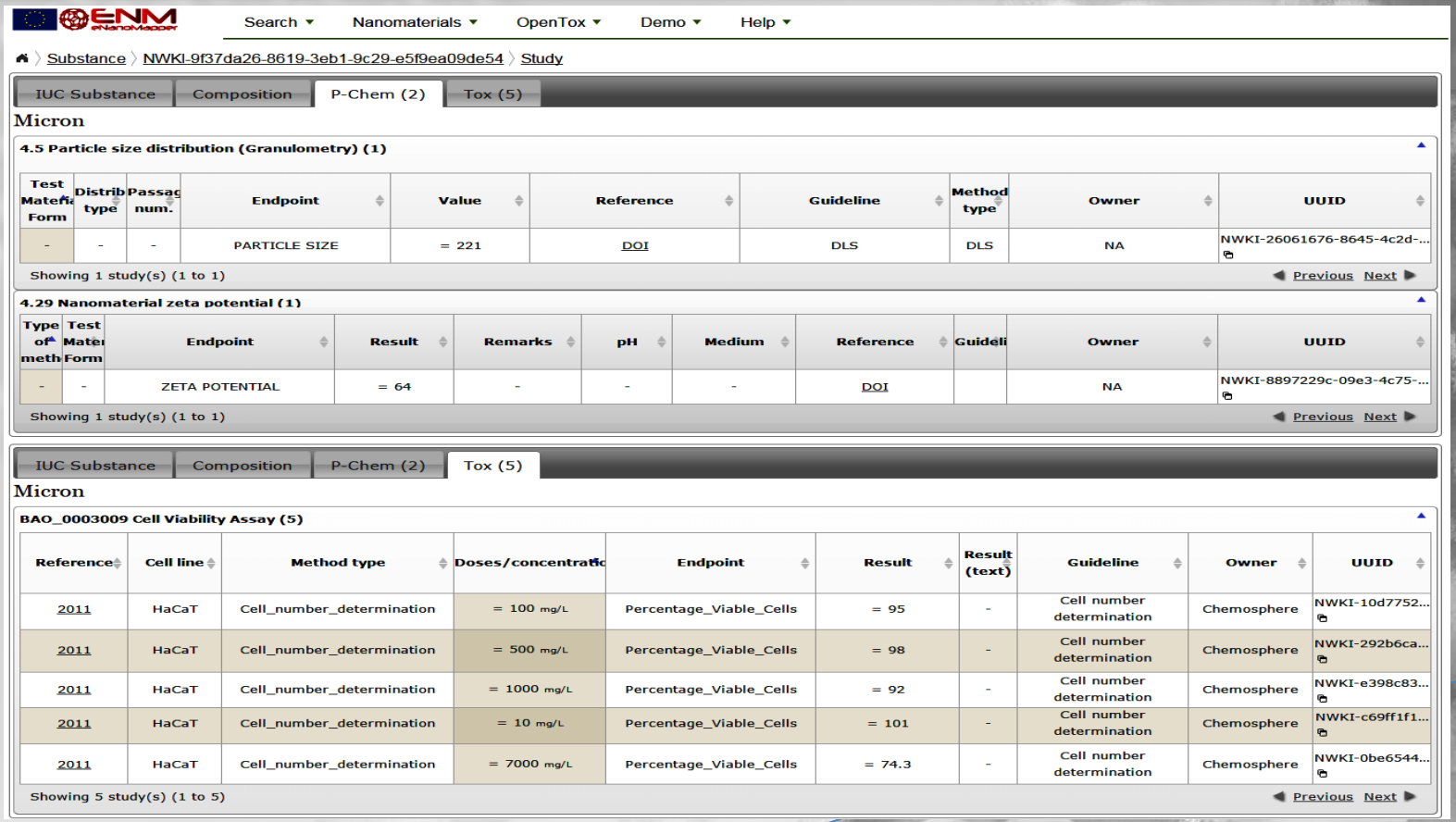
Parameters

Parameter	Value	Description	Parameter Type	Data Type
title			form	string
description			form	string
dataset_uri	op.jaqpot.org:8080/jaqpot/services/dataset/corona		form	string
prediction_feature	https://apps.ideaconsult.net/enmtest/property/TOX		form	string
parameters			form	string
transformations	http://app.jaqpot.org:8080/jaqpot/services/pmml/cc		form	string
scaling			form	string
doa	http://app.jaqpot.org:8080/jaqpot/services/algorithr		form	string
id	ocpu-lm		path	string
subjectid			header	string

Try it out!

eNanoMapper

Prototype database:
Phys chem & Tox (NanoWiki)



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Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

Substance 〉 NWKI-9f37da26-8619-3eb1-9c29-e5f9ea09de54 〉 Study

IUC Substance | Composition | P-Chem (2) | Tox (5)

Micron

4.5 Particle size distribution (Granulometry) (1)

Test Materi Form	Distrib type	Passag num.	Endpoint	Value	Reference	Guideline	Method type	Owner	UUID
-	-	-	PARTICLE SIZE	= 221	DOI	DLS	DLS	NA	NWKI-26061676-8645-4c2d-...

Showing 1 study(s) (1 to 1) ◀ Previous Next ▶

4.29 Nanomaterial zeta potential (1)

Type of meth	Test Mater Form	Endpoint	Result	Remarks	pH	Medium	Reference	Guideli	Owner	UUID
-	-	ZETA POTENTIAL	= 64	-	-	-	DOI		NA	NWKI-8897229c-09e3-4c75-...

Showing 1 study(s) (1 to 1) ◀ Previous Next ▶

IUC Substance | Composition | P-Chem (2) | Tox (5)

Micron

BAO_0003009 Cell Viability Assay (5)

Reference	Cell line	Method type	Doses/concentratic	Endpoint	Result	Result (text)	Guideline	Owner	UUID
2011	HaCaT	Cell_number_determination	= 100 mg/L	Percentage_Viable_Cells	= 95	-	Cell number determination	Chemosphere	NWKI-10d7752...
2011	HaCaT	Cell_number_determination	= 500 mg/L	Percentage_Viable_Cells	= 98	-	Cell number determination	Chemosphere	NWKI-292b6ca...
2011	HaCaT	Cell_number_determination	= 1000 mg/L	Percentage_Viable_Cells	= 92	-	Cell number determination	Chemosphere	NWKI-e398c83...
2011	HaCaT	Cell_number_determination	= 10 mg/L	Percentage_Viable_Cells	= 101	-	Cell number determination	Chemosphere	NWKI-c69ff1f1...
2011	HaCaT	Cell_number_determination	= 7000 mg/L	Percentage_Viable_Cells	= 74.3	-	Cell number determination	Chemosphere	NWKI-0be6544...

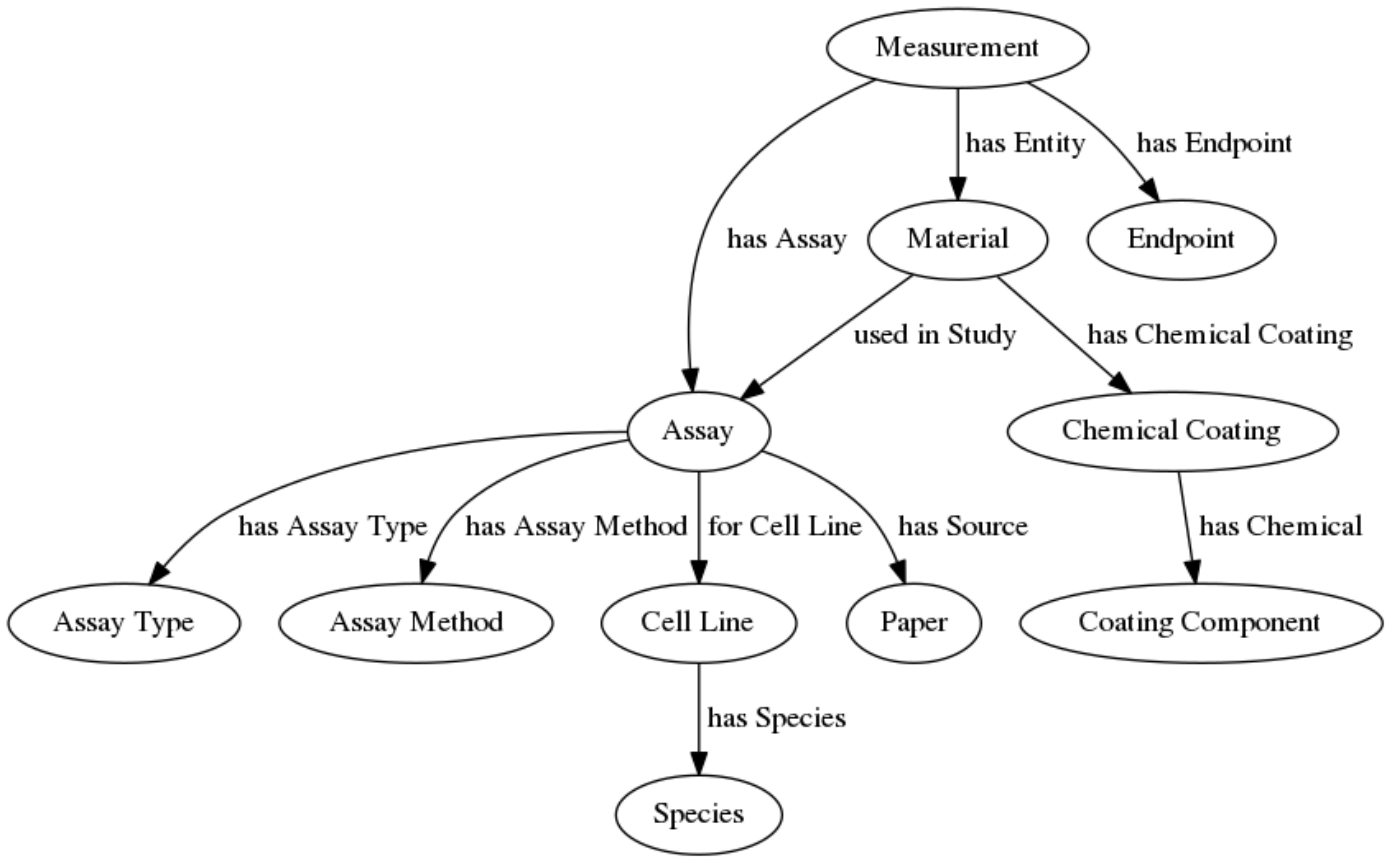
Showing 5 study(s) (1 to 5) ◀ Previous Next ▶

eNM eNanoMapper

Importing data: NanoWiki

- Export data from an existing database
- Import data into the eNM platform
- Test if it works

NanoWiki Structure



Imported into eNanoMapper

IUC Substance | Composition | P-Chem (6)

Filter...

Expand all | Collapse all

PNP26

4.5 Particle size distribution (Granulometry) (1)

Test Material Form	Distributi type	Endpoint	Value	Reference	Guideline	Owner	UUID
-	-	PARTICLE SIZE	= 20	DOI		-	NWKI-3dd176d2-8...

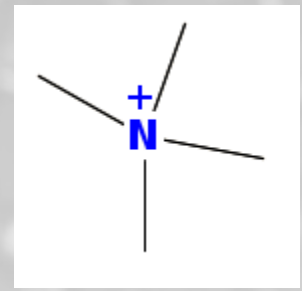
Showing 1 study(s) (1 to 1) Previous Next

4.29 Nanomaterial zeta potential (1)

Type of method	Test Material Form	Endpoint	Result	Reference	Guideline	Owner	UUID
-	-	ZETA POTENTIAL	= -4.3	DOI		-	NWKI-3cbe101f-b...

eNanoMapper

Chemical substructure search



Search | Nanomaterials | OpenTox | Demo | Help | Log

Search structures and associated data

Exact structure | Similarity | Substructure | URL

Cationic (quaternary ammor | [N+](*)(*)(*)*

Identifiers | Datasets | Export

Showing from 1 to 4 in pages of 20 entries Previous Next

	Diagram	CAS	EINECS	Name	Trade Name	IUPAC Name	SMIL	REACH Date	Similarity
- 1 -					-	-	-	-	-
- 2 -					-	-	-	-	-

Azides
Benzotriazoles
Benzotriazoles
Boron Compounds
Boron Compounds (borates and borate esters)
Boron Compounds (organoboranes)
Boron Compounds (organoboranes)
Boron Compounds (boroxines)
Boron Compounds (boroxines)
Boron Compounds (boron hydride)
Boron Compounds (boron hydride)
Cationic (quaternary ammonium) surfactants
Cationic (quaternary ammonium) surfactants
Cobalt
Cobalt
Diazoniums
Diazoniums
Dichlorobenzidine-based Pigments
Dichlorobenzidine-based Pigments
Dithiocarbamates

Identifiers | Substances

	Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info	Contained in as
- 1 -	S40.MUTA	FCSV-1f4...	nanoparticle	S40.MUTA	FCSV-9a...	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic	coating
- 2 -	G30.MUTA	FCSV-3a...	nanoparticle	G30.MUTA	FCSV-50...	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic	coating
- 3 -	G60.MUTA	FCSV-8e...	nanoparticle	G60.MUTA	FCSV-50...	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver	Classification = Cationic	coating

Identifiers | Substances

	Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info	Contained in as
- 1 -	Harper2011 6	NWKI-36...	Metal	Ag	NWKI-36...	NanoWiki	Coating = TMATCoating Composition = Ag DATASET = NanoWiki Has_Identifier = 96	coating
- 2 -	Harper2011 3	NWKI-e8...	Metal	Ag	NWKI-e8...	NanoWiki	Coating = TMATCoating Composition = Ag DATASET = NanoWiki Has_Identifier = 93	coating
- 3 -	Harper2011 7	NWKI-fe...	Metal	Ag	NWKI-fe...	NanoWiki	Coating = TMATCoating Composition = Ag DATASET = NanoWiki Has_Identifier = 97	coating

Coating

Protein Corona dataset

NanoWiki

eNanoMapper

NanoEHS – EU-US Communities of Research

1. Exposure
2. Eco Toxicity
3. Risk Assessment
4. Risk Management
5. Human Health
6. Data and Modelling
7. Characterisation

Encourage joint programs of work that leverage EU and US resources.

eNanoMapper

Project partners

Douglas Connect
Working communities

in silico toxicology

IOFA consult

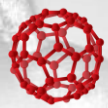
Karolinska Institutet

VTT

EMBL-EBI

Maastricht University

misvik biology



eNanoMapper

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Jeliazkova N, Chomenidis C, Doganis P, Fadeel B, Grafström R, Hardy B, Hastings J, Hegi M, Jeliazkov V, Kochev N, Kohonen P, Munteanu CR, Sarimveis H, Smeets B, Sopasakis P, Tsiliki G, Vorgrimmler D, Willighagen E. *The eNanoMapper database for nanomaterial safety information*. Beilstein Journal of Nanotechnology, **2015** [*in press*]

Hastings J, Jeliazkova N, Owen O, Tsiliki G, Munteanu CR, Steinbeck C, Willighagen E. *eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment*, Journal of Biomedical Semantics, **2015**, 6:10

Hastings J, Willighagen E, Owen G, Jeliazkova N, Steinbeck C. *eNanoMapper: Opportunities and challenges in using ontologies to enable data integration for nanomaterial risk assessment*. In Proceedings of the ISMB Bio-Ontologies SIG meeting, Boston, USA, July 11-12 **2014**.

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eNM eNanoMapper

FP7-eNanoMapper

"eNanoMapper - A Database and Ontology Framework for Nanomaterials Design and Safety Assessment"

- Grant Agreement: 604134
- Duration: 36 months (1 Feb 2014 – 31 Jan 2016)