

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 be taken as indicating any official position of any organisation.

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www.enanomapper.net

Collaborating Partners on eNanoMapper

Douglas Connect,
Switzerland
(Coordinator)

Maastricht University,
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In Silico
Toxicology,
Switzerland

National Technical
University of Athens,
Greece

Ideaconsult,
Bulgaria



EMBL-EBI, UK

Karolinska
Institutet,
Sweden

VTT, Finland

Associate Partners



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)

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

OpenTox and Open Components and Standards

<-New API addition from ToxBank

Investigation (Study, Assay)

GET
POST
PUT
DELETE

Authorisation & Authentication

GET
POST
PUT
DELETE

AppDomain

GET
POST
PUT
DELETE

Report

GET
POST
PUT
DELETE

Dataset

GET
POST
PUT
DELETE

Validation

GET
POST
PUT
DELETE

Feature

GET
POST
PUT
DELETE

Compound

GET
POST
PUT
DELETE

Model

GET
POST
PUT
DELETE

Ontology

GET
POST
PUT
DELETE

Algorithm

GET
POST
PUT
DELETE

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 Jeliaskova (Ideacon), 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



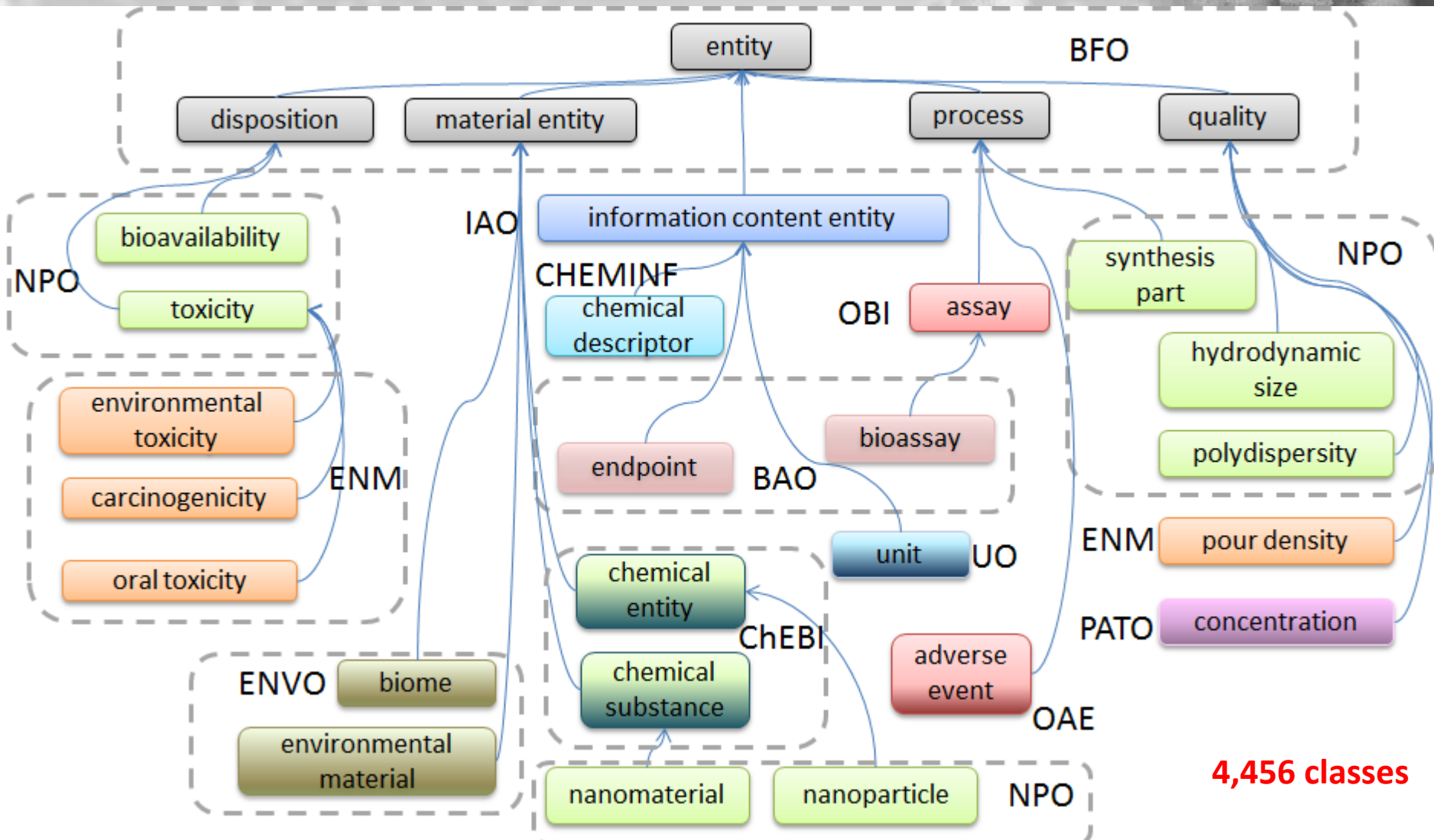
Prototype eNanoMapper ontology

The screenshot displays the eNanoMapper ontology editor interface. The main window shows the ontology file path: `enanomapper (http://purl.enanomapper.org/onto/enanomapper.owl) : [C:\Work\Ontologies\enanomapper\ontologies\enanomapper.owl]`. The interface includes a menu bar (File, Edit, View, Reasoner, Tools, Refactor, Window, Help) and a toolbar with navigation and search options. The central area is divided into several panes:

- Class hierarchy:** Shows a tree structure starting with `Thing` and `entity`. Under `entity`, there are several classes including `disposition`, `toxicity`, and `environmental toxicity`. The `environmental toxicity` class is currently selected and highlighted.
- Annotations:** Shows the annotations for the selected class, including a `label` (language: en) with the value `environmental toxicity` and a `definition` with the value `Toxicity to some part or aspect of the environment.`
- Description:** Shows the description for the selected class, including `Equivalent To`, `SubClass Of` (with `toxicity` listed), and `SubClass Of (Anonymous Ancestor)`.

At the bottom of the interface, there is a status bar with the text: `To use the reasoner click Reasoner->Start reasoner` and a checked checkbox for `Show Inferences`.

Ontology assembled from multiple sources



- intensity
- mass
- 'mass density'
- 'particle size'
- 'physical state'
- polydispersity
 - 'molecular weight distribution'
 - monodisperse
 - polydisperse
 - 'size distribution'
 - 'particle size distribution'
- porosity
- 'pour density'

topObjectProperty

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>
```

Equivalent To +

SubClass Of +

'size distribution'

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/enanomappper/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](#)



bioportal.bioontology.org/ontologies/ENM



Browse classes

eNanoMapper

Summary **Classes** Properties Notes Mappings Widgets

Jump To:

- entity
 - disposition
 - information content entity
 - material entity
 - process
 - adverse event
 - assay
 - functionalization of nanoparticle
 - synthesis part
 - quality

Details	Visualization	Notes (0)	Class Mappings ()
Preferred Name		entity	
ID		http://purl.obolibrary.org/obo/BFO_0000001	
editor preferred label		entity	
label		entity	
prefixIRI		BFO:0000001	
prefLabel		entity	
subClassOf		http://www.w3.org/2002/07/owl#Thing	

View metadata (synonyms, ID)

eNanoMapper

Summary Classes Properties Notes Mappings Widgets

Jump To:

- entity
 - disposition
 - information content entity
 - material entity
 - process
 - quality
 - concentration of
 - dustiness
 - hydrodynamic size
 - intensity
 - mass
 - mass density
 - particle size
 - physical state
 - polydispersity
 - molecular weight distribution
 - monodisperse
 - polydisperse
 - size distribution**

Details

Visualization

Notes (0)

Class Mappings (2)



Preferred Name	size distribution
ID	http://purl.bioontology.org/ontology/npo#NPO_1697
code	NPO_1697
definition	A polydispersity inhering in a collection of objects based on size.1
FULL_SYN	size distributionPTNCI
label	size distribution
preferred_name	size distribution
prefixIRI	npo:NPO_1697
prefLabel	size distribution
subClassOf	polydispersity

eNanoMapper Ontology in Protegé

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

The screenshot displays the Protegé web interface for the eNanoMapper ontology. The browser address bar shows the URL <http://purl.enanomapper.org/onto/enanomapper.owl>. The interface includes a navigation menu with options like Active Ontology, Entities, Classes, Object Properties, Data Properties, Annotation Properties, Individuals, OWLViz, DL Query, OntoGraf, SPARQL Query, and Ontology Differences. The main content area is divided into sections: Ontology header, Annotations, and Ontology metrics.

Ontology header:

- Ontology IRI: <http://purl.enanomapper.org/onto/enanomapper.owl>
- Ontology Version IRI: e.g. <http://purl.enanomapper.org/onto/enanomapper.owl/1.0.0>

Annotations:

- Contributor:** Nina Jeliaskova
- comment:** 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. This ontology is an application ontology targeting the full domain of nanomaterial safety assessment. It re-uses several other ontologies including the NPO, CHEMINF, ChEBI, and ENVO.
- license:** CC-BY 3.0 <https://creativecommons.org/licenses/by/3.0/>
- Contributor:** Gareth Owen
- Contributor:** Janna Hastings

Ontology metrics:

Metrics	
Axiom	48483
Logical axiom count	5910

Imported ontologies:

- Ontology imports
- Ontology Prefixes
- General class axioms

Browse, Search

The screenshot displays the ENM web interface. The browser address bar shows the URL `http://purl.enanmapper.org/onto/enanmapper.owl`. The 'Classes' tab is selected in the top navigation bar. On the left, the 'Class hierarchy' for 'epigenetic modification assay' is shown, with 'epigenetic modification assay' highlighted. The right panel shows the 'Annotations' for this class, including a label, definition, and source. The 'Description' panel below shows that 'epigenetic modification assay' is a subclass of 'assay'.

enanomapper (http://purl.enanmapper.org/onto/enanmapper.owl) : [http://purl.enanmapper.org/onto/enanmapper.owl]

enanomapper (http://purl.enanmapper.org/onto/enanmapper.owl) Search for entity

Active Ontology Entities **Classes** Object Properties Data Properties Annotation Properties Individuals OWLviz DL Query OntoGraf SPARQL

Class hierarchy Class hierarchy (inferred)

Class hierarchy: 'epigenetic modification assay'

- entity
 - disposition
 - 'information content entity'
 - 'material entity'
 - process
 - 'adverse event'
 - assay
 - 'activated partial thromboplastin tir
 - 'age measurement assay'
 - 'analyte assay'
 - 'array based nucleic acid structure
 - 'assay detecting IFN-gamma produ
 - 'assay for transposase-accessible ct
 - 'B cell epitope specific neutralization
 - 'Bernoulli trial'
 - 'binding assay'
 - bioassay
 - 'cell mediated cell killing assay'
 - 'cell proliferation assay'
 - 'comet assay'
 - 'copy number variation profiling'
 - 'cytochalasin-induced inhibition of
 - 'detection of molecular label'
 - 'DNA replication timing by array as
 - 'DNA sequence feature detection'
 - 'DNA sequence variation detection'
 - 'efficacy of epitope intervention exp
 - 'ELISPOT assay'
 - 'epigenetic modification assay'
 - 'extracellular electrophysiology rec

Annotations: 'epigenetic modification assay'

Annotations +

- label
 - epigenetic modification assay
- definition
 - An assay that identifies epigenetic modification including histone modifications, open chromatin, and DNA methylation.
- 'definition source'
 - Penn group
- 'editor preferred term'
 - epigenetic modification assay
- 'has curation status'
 - 'metadata complete'
- Source
 - Beta Cell Biology Consoritum

Description: 'epigenetic modification assay'

Equivalent To +

SubClass Of +

- assay

SubClass Of (Anonymous Ancestor)

Logic-based querying

DL query:

Query (class expression)

bioassay **and** 'has endpoint' **some** 'concentration endpoint'

Execute

Add to ontology

Query results

Sub classes (2)

● 'KiNativ assay'

?

GitHub enanomapper ontologies

enanomapper / ontologies

Watch 15 Star 0 Fork 1

Issues Pull requests Labels Milestones

Filters is:issue is:open New issue

<input type="checkbox"/>	21 Open ✓ 4 Closed	Author	Labels	Milestones	Assignee	Sort
<input type="checkbox"/>	Incorporation of several URIs from new and already used ontology resources #25 opened 6 days ago by Irieswijk					0
<input type="checkbox"/>	endpoints to be added #24 opened 28 days ago by vedina					0
<input type="checkbox"/>	NM_001005 describes both particle size and zeta potential ENM #23 opened 28 days ago by vedina					4
<input type="checkbox"/>	protocol and assay type entries #22 opened 29 days ago by vedina					1
<input type="checkbox"/>	Add National Cancer Institute Thesaurus to ontology #21 opened 29 days ago by Irieswijk					0
<input type="checkbox"/>	Merge 'toxicity' and 'toxicity endpoint' branches #20 opened on May 13 by jannahastings					2
<input type="checkbox"/>	include STATO for e.g. min/max #19 opened on May 12 by jannahastings					1

Navigation icons: <>, ⓘ, 🔗, 📖, 🔊, 📊, 🛠️

REST Application Programming Interface

API documentation (Swagger-UI)

The screenshot shows the Swagger-UI for the eNanoMapper prototype database API. The page title is "eNanoMapper prototype database API" and it provides a description of the API and links to terms of service, developer contact, and license. A list of services is shown, including OpenTox Algorithms, Chemical Compounds, Dataset, Feature, Prediction Models, Properties, Queries, Structures search, and Substance search. The "substance : Chemical Substances service" is expanded to show a list of endpoints with their methods and descriptions:

- GET /substance: List substances
- POST /substance: Import substance(s) and studies
- GET /substance/{uuid}: Get a substance
- GET /substance/{uuid}/composition: Get substance composition
- GET /substance/{uuid}/structures: Get substance composition as a dataset
- GET /substance/{uuid}/study: Get substance study
- GET /substance/{uuid}/studysummary: Get study summary for the substance

At the bottom, the base URL is given as <https://apps.ideaconsult.net/enanomapper/api-docs> and the API version is 2.7.2.

Interactive API queries

The screenshot shows the interactive API query interface for the "substance : Chemical Substances service". It displays a list of endpoints with their methods and descriptions. The "GET /substance/{uuid}/study" endpoint is selected, and the response is shown in a JSON format:

```
{
  "interpretation": "object",
  "owner": "object",
  "parameters": "object",
  "protocol": "object",
  "reliability": "object",
  "units": ""
}
```

The interface also shows a table of parameters for the selected endpoint:

Parameter	Value	Description	Parameter Type	Data Type
uuid	NWKI-02981d44-b7d0-34c8-abab-d419a5a40865	Substance UUID	path	string
top	P-CHEM	Top endpoint category	query	string
category		Endpoint category (the value in the protocol category code field)	query	string
property		Property UUID	query	string
property_url		Property URL https://apps.ideaconsult.net/enmtest/property/{UUID} . see Property service	query	string
page	0	Starting page	query	int
pagesize	10	Page size	query	int

Below the parameters table, there is a "Response Messages" section showing HTTP status codes and reasons. The "Request URL" is <https://apps.ideaconsult.net:443/enmtest/substance/NWKI-02981d44-b7d0-34c8-abab-d419a5a40865/study?top=P-CHEM&page=0&pageSize=10>. The "Response Body" is shown in a JSON format:

```
{
  "TESTRESULT_FORM": null
},
{
  "reliability": {
    "is_substudy": "false",
    "is_listed_for_classification": "false",
    "is_listed_for_om": "false",
    "is_purpose_driven": "false",
    "is_purpose_driven": "false",
    "study_result_type": "experimental result",
    "value": null
  },
  "interpretation": {
    "result": null
  },
  "effects": {
    {
      "endpoint": "PARTICLE SIZE",
      "conditions": {},
      "result": {
        "unit": "nm",
        "value": 20
      }
    }
  }
}
```

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

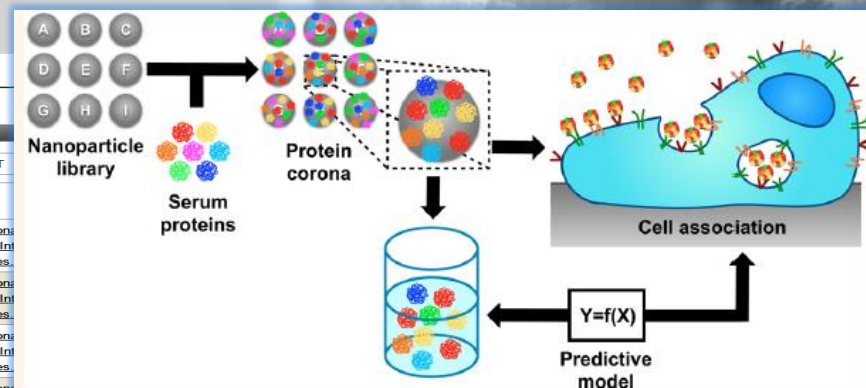
Prototype database (NM components)

ENM eNanoMapper Search Nanomaterials OpenTox Demo Help

Search substances by identifiers

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

Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID		
- 11 -	G15.DDT@BDHDA	FCSV-2a85f394...	nanoparticle	G15.DDT@BDHDA	FCSV-2a85f394...	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



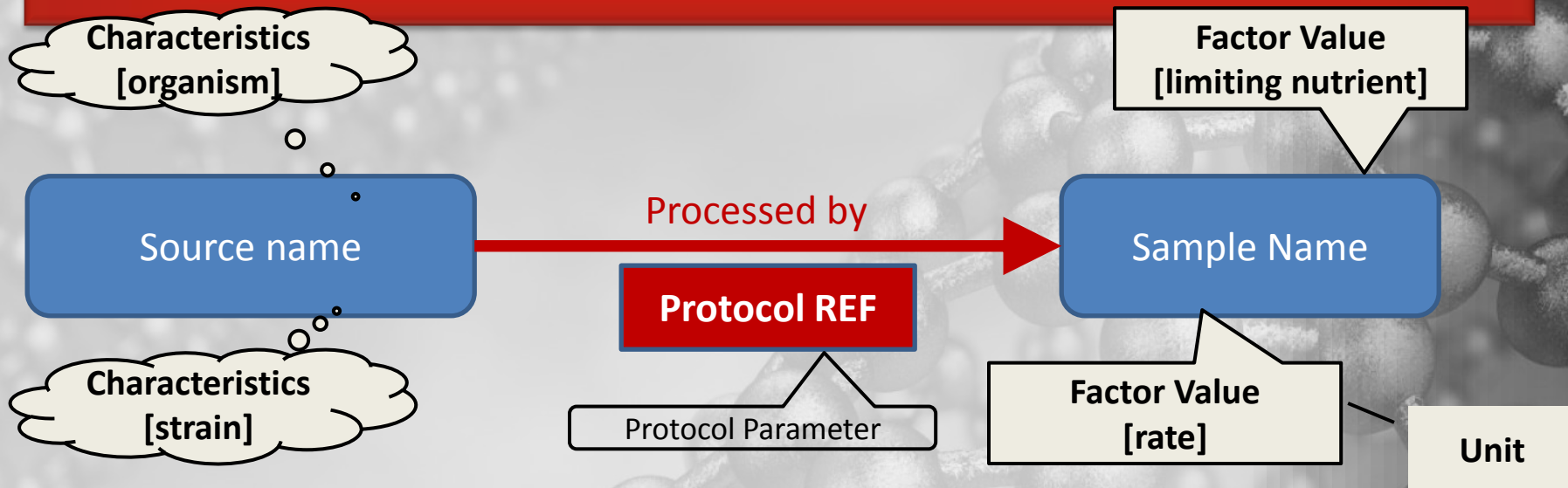
Protein Corona Data set
DOI:10.1021/nn406018q

Composition name: FCSV-fb5e6048-8ee1-351d-915b-d1669681357e
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,Wnahlzmsdqwp-Uhfffoa-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
Coating	Octadecan-1-Amine,Reyjsvuryzge-Uhfffoa-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
Core	[Au]			0 % (w/w)	0 % (w/w) 0 % (w/w)	Also contained

Search:

- 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



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

ambit ENM Search ▾ D

Search substances by endpoint data

Update results

P-Chem

- 4.2. Melting point / freezing point (1) [2]
- 4.24. Nanomaterial agglomeration/aggregation (1) [1]
- 4.25. Nanomaterial crystalline phase (1) [1]
- 4.26. Nanomaterial crystallite and grain size (526) [526]
- 4.27. Nanomaterial aspect ratio/shape (1) [1]
- 4.28. Nanomaterial specific surface area (1) [1]
- 4.29. Nanomaterial zeta potential (612) [618]
- 4.3. Boiling point (1) [2]
- 4.30. Nanomaterial surface chemistry (604) [1209]
- 4.31. Nanomaterial dustiness (1) [1]
- 4.32. Nanomaterial porosity (1) [1]
- 4.33. Nanomaterial pour density (1) [1]
- 4.34. Nanomaterial photocatalytic activity (1) [1]
- 4.36. Nanomaterial catalytic activity (1) [1]
- 4.5. Particle size distribution (Granulometry) (Z18) [1265]
- 4.7. Partition coefficient (1) [2]
- 4.8. Water solubility (1) [1]

Endpoint name Units

Core size nm

Value

>= ▾ 59 <= ▾ 60

Update results

Env Fate

Eco Tox

Tox

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	UUID
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						
			Volume Mean Hydrodynamic Diameter	= 244.57 nm						
			Number Mean Hydrodynamic Diameter	= 87.28 nm						
			Number Mean Hydrodynamic Diameter	= 88.72 nm						
			Intensity Mean Hydrodynamic Diameter	= 87.28 nm						
			Intensity Mean Hydrodynamic Diameter	= 121.04 nm						
TEM	-		Core size	mean 59.3 nm	-	doi: 10.1021/nn4060	2014	-	Tecnai 20 (FEI) microscop	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](#)

Protocol service

ENM eNanoMapper

Protocol User management Admin Help [nina] Log out

Protocols

Showing 15 protocols (1 to 10)

Identifier	Title	Status / Owner	Abstract	Project	Organisation	Updated
ENMNSC-Protocol-1-1	Comet Assay Published: Yes Download	RESEARCH Owner	This protocol describes the single cell gel electrophoresis assay (also known as the Comet assay) which is a simple, rapid and sensitive technique for analysing and quantifying DNA damage in individual mammalian (and to some extent prokaryotic) cells. This was first introduced by Ostling and Johanson in 1984. This was a neutral assay in which the lysis and electrophoresis were done under neutral conditions. Staining was done with acridine orange. The image obtained looked like a "comet" with a distinct head comprising of intact DNA and a tail, consisting of damaged or broken pieces of DNA hence the name. The more versatile alkaline method of the comet assay was given by Singh and co workers in 1988. This method was developed to measure DNA damage breaks with high sensitivity.	ENPRA	Institute of Anatomy, Division of Histology, University of Bern	Tue Jan 27 2015
ENMNSC-Protocol-10-1	Development of a Particle Size Sampler for Biological Exposure Studies Published: Yes Download	RESEARCH Owner	In this study, a Selective Particle Size (SPS) sampler was developed, which is able to provide continuous delivery of diesel soot particles of specific size ranges. The SPS sampler, it is possible to obtain two aerosol streams with different size distributions, suitable for biological exposure studies. A cell exposure protocol is described here.			
ENMNSC-Protocol-11-1	Detecting HO-1 and IL8 by q-PCR Published: Yes Download	RESEARCH Owner	The protocol describes the method to detect HO-1 and IL8 by quantitative real-time PCR.			
ENMNSC-Protocol-12-1	Detection and semi-quantification of Endotoxin Contaminations in NanoParticle Suspensions Published: Yes Download	RESEARCH Owner	In vitro endotoxin test for the detection and semi-quantification of endotoxin in aqueous nanoparticle suspensions using Limulus amoebocyte lysate (LAL) test.			
ENMNSC-Protocol-13-1	Profiling of the nanomaterial-protein corona Published: Yes Download	RESEARCH Owner	Due to their high free surface energy, most likely all nanomaterials adsorb proteins upon contact with any (biological) fluid. In particular, proteins rapidly adsorb to nanoparticles forming a biological coating around the nanoparticle known as the protein corona. Hence, "naked" nanomaterials in general are expected to behave differently in biological environments only for a short time (< 1min). Therefore, the biomolecular corona of nanomaterials need to be considered as novel materials with different properties compared to the pristine nanomaterials during their manufacturing. Particularly, the protein corona interacts with biological systems and thus, constitutes a major element of the nanomaterial identity. As such, the protein corona will also influence the nanotoxicology, including ecotoxicology, and may influence success of nanomedicine applications.			

Search:

github.com/enanomapper

Search GitHub

Explore Gist Blog Help

eNanoMapper

Funded from the European Union's FP7 for research, technological development and demonstration under grant agreement no 604134.

http://enanomapper.net/

Filters Find a repository... + New repository

nmdataparser Java ★ 0

Parsers for different NM data formats

Updated 19 minutes ago

toxbank-api-server Java ★ 0

Forked from ToxBank/toxbank-api-server

ToxBank Protocol service

Updated 5 days ago

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

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.

Modelling Infrastructure

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

 **Jaqpote Quattro** <http://enanomapper.ntua.gr:8880/jaqpot/services/api-d> [AQIC5wM2LY4SfczIqjwPxhwl](#) [Explore](#)

dataset : Dataset API	Show/Hide	List Operations	Expand Operations	Raw
pmmi : PMML API	Show/Hide	List Operations	Expand Operations	Raw
bibtex : BibTeX API	Show/Hide	List Operations	Expand Operations	Raw
enanomapper : eNM API	Show/Hide	List Operations	Expand Operations	Raw
model : Models API	Show/Hide	List Operations	Expand Operations	Raw
task : Tasks API	Show/Hide	List Operations	Expand Operations	Raw
algorithm : Algorithms API	Show/Hide	List Operations	Expand Operations	Raw
aa : AA API	Show/Hide	List Operations	Expand Operations	Raw
feature : Feature API	Show/Hide	List Operations	Expand Operations	Raw
user : Users API	Show/Hide	List Operations	Expand Operations	Raw

[BASE URL: <http://enanomapper.ntua.gr:8880/jaqpot/services/api-docs>]

Modelling Infrastructure

Image Analysis Application

Select the threshold type:

Descriptors:

- | | | | | | |
|---|---|---|--|---|--|
| <input type="checkbox"/> Area | <input type="checkbox"/> Porosity | <input type="checkbox"/> Bounding Preferences | <input type="checkbox"/> Center of mass | <input type="checkbox"/> Centroid | <input type="checkbox"/> Feret |
| <input type="checkbox"/> Fit Ellipse | <input type="checkbox"/> Integrated Density | <input type="checkbox"/> Kurtosis | <input type="checkbox"/> Mean Gray Value | <input type="checkbox"/> Median | <input type="checkbox"/> Minimum and Maximum |
| <input type="checkbox"/> Modal Gray Value | <input type="checkbox"/> Perimeter | <input type="checkbox"/> Shape Descriptors | <input type="checkbox"/> Skeweness | <input type="checkbox"/> Standard Deviation | <input type="checkbox"/> Sphericity |
| <input type="checkbox"/> Particle Volume Estimation | <input type="checkbox"/> Surface Diameter | <input type="checkbox"/> Volume to Surface | <input type="checkbox"/> Volume Diameter | | |

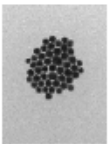
Image Preview



+ Choose a file or drag and drop it here

Upload

Cancel



example image.jpg 2.4 MB



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	<input type="text"/>		form	string
description	<input type="text"/>		form	string
dataset_uri	<input type="text" value="bp.jaqpot.org:8080/jaqpot/services/dataset/corona"/>		form	string
prediction_feature	<input type="text" value="https://apps.ideaconsult.net/enmtest/property/TOX"/>		form	string
parameters	<input type="text"/>		form	string
transformations	<input type="text" value="http://app.jaqpot.org:8080/jaqpot/services/pmm/cc"/>		form	string
scaling	<input type="text"/>		form	string
doa	<input type="text" value="http://app.jaqpot.org:8080/jaqpot/services/algorithm"/>		form	string
id	<input type="text" value="ocpu-lm"/>		path	string
subjectid	<input type="text"/>		header	string

Try it out!

```
app.jaqpot.org:8080/jaqpot/services/dataset/JYKC24AkXw5Koa
app.jaqpot.org:8080/jaqpot/services/...
1- [
2-   "meta": {
3-     "comments": [
4-       "Created by task TSK1z3000eQEYC5"
5-     ],
6-     "creators": [
7-       "guest"
8-     ],
9-     "hasSources": [
10-      "https://apps.ideaconsult.net/enmtest/bundle/28"
11-    ]
12-  },
13-  "datasetURI": "http://app.jaqpot.org:8080/jaqpot/services/dataset/szu95fY88CuTa9",
14-  "dataEntry": [
15-    {
16-      "compound": {
17-        "URI": "FC5V-0929e367-b24a-3938-b089-e543321e3832"
18-      },
19-      "values": {
20-        "Predicted feature
21-        "http://app.jaqpot.org:8080/jaqpot/services/Feature/7nza0J2AbbKJ": -5.8421,
22-        "http://app.jaqpot.org:8080/jaqpot/services/Feature/EzYREKj6FkNm": -17.349999999999998,
23-        "http://app.jaqpot.org:8080/jaqpot/services/Feature/Im9BUqz38aVY": 3.578008915304606,
24-        "http://app.jaqpot.org:8080/jaqpot/services/Feature/AZDc11TA1A": 0.7549819163291235,
25-        "http://app.jaqpot.org:8080/jaqpot/services/Feature/LSGGFLXGUpF": 24.08,
26-        "http://app.jaqpot.org:8080/jaqpot/services/Feature/prWRZOTcCKD": 6.73,
27-        "https://apps.ideaconsult.net/enmtest/property/TOX/UNKNOWN_TOXICITY_SECTION/Log2+transformed/940664CFE4929A0F400ASAD8CA733852E049A688/3ed642f9-1b42-387a-9966-dea5b91e5f8a": -5.505
28-      }
29-    }
30-  ]
31-}
```

Prototype database: Phys chem & Tox (NanoWiki)

ENM eNanoMapper

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 Material 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 Material meth 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/concentrat	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](#)

Importing data: NanoWiki

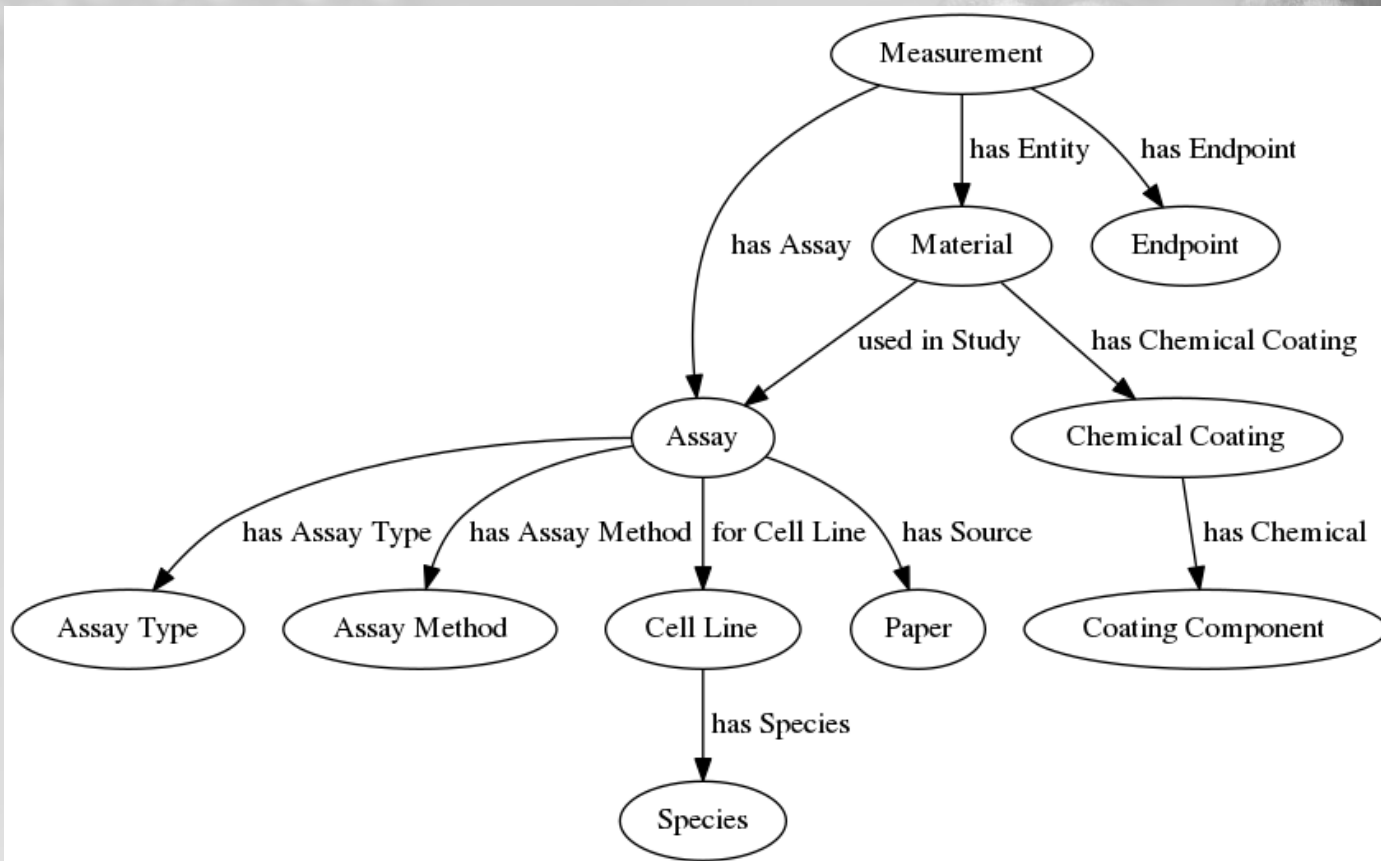
- Export data from an existing database
- Import data into the eNM platform
- Test if it works

Facts about Liu2011Cytotox ⓘ

RDF feed 

For Cell line	BEAS-2B + 
Has Assay Method	PI uptake assay + 
Has Assay Type	Cell Viability Assay + 
Has Entities	MetalOxides + 
Has Identifier	3 + 
Has Source	Liu2011 + 

NanoWiki Structure



Imported into eNanoMapper

IUC Substance Composition **P-Chem (6)**

Filter... Expand all Collapse all

PNP26

4.5 Particle size distribution (Granulometry) (1)

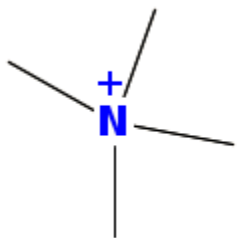
Test Material Form	Distributi type	Endpoint	Value	Reference	Guideline	Owner	UUID
-	-	PARTICLE SIZE	= 20	DOI		-	NWKI-3dd176d2-8...

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...

Chemical substructure search



ENM Search Nanomaterials OpenTox Demo Help

Search structures and associated data

Exact structure Similarity Substructure URL

Identifiers Datasets

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

Diagram CAS EINECS Name Trade Name IUPAC Name SMIL

REACH Date Similarity

Export

Cationic (quaternary ammonium) surfactants

Coating

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	NWKL-36...	Metal	Ag	NWKL-36...	NanoWiki	Coating = TMATCoating Composition = Ag DATASET = NanoWiki Has_Identifier = 96	coating
- 2 -	Harper2011 3	NWKL-e8...	Metal	Ag	NWKL-e8...	NanoWiki	Coating = TMATCoating Composition = Ag DATASET = NanoWiki Has_Identifier = 93	coating
- 3 -	Harper2011 7	NWKL-fe...	Metal	Ag	NWKL-fe...	NanoWiki	Coating = TMATCoating Composition = Ag DATASET = NanoWiki Has_Identifier = 97	coating

Protein Corona dataset

NanoWiki

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.

Project partners

Douglas Connect
Working communities



in silico toxicology

IOFA
consult



Karolinska
Institutet



EMBL-EBI



Maastricht University

misvik biology



References

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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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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)