

The first eNanoMapper prototype: a substance database to support a safe innovation approach



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FP7 eNanoMapper project

- Started Feb 2014, 3 years
- Develop an ontology and database unifying information about nanomaterial safety (in humans and the environment)
- Cover the full lifecycle from manufacturing to environmental decay or accumulation
- Pan-European project, 8 partners
- Ontology growth through community and re-use

Objective: Safety by Design



Maastricht University *Leading in Learning!*

EMBL-EBI



Douglas Connect GmbH



IQFA
consult



**Nat. Tech. Univ. of
Athens, Greece —**

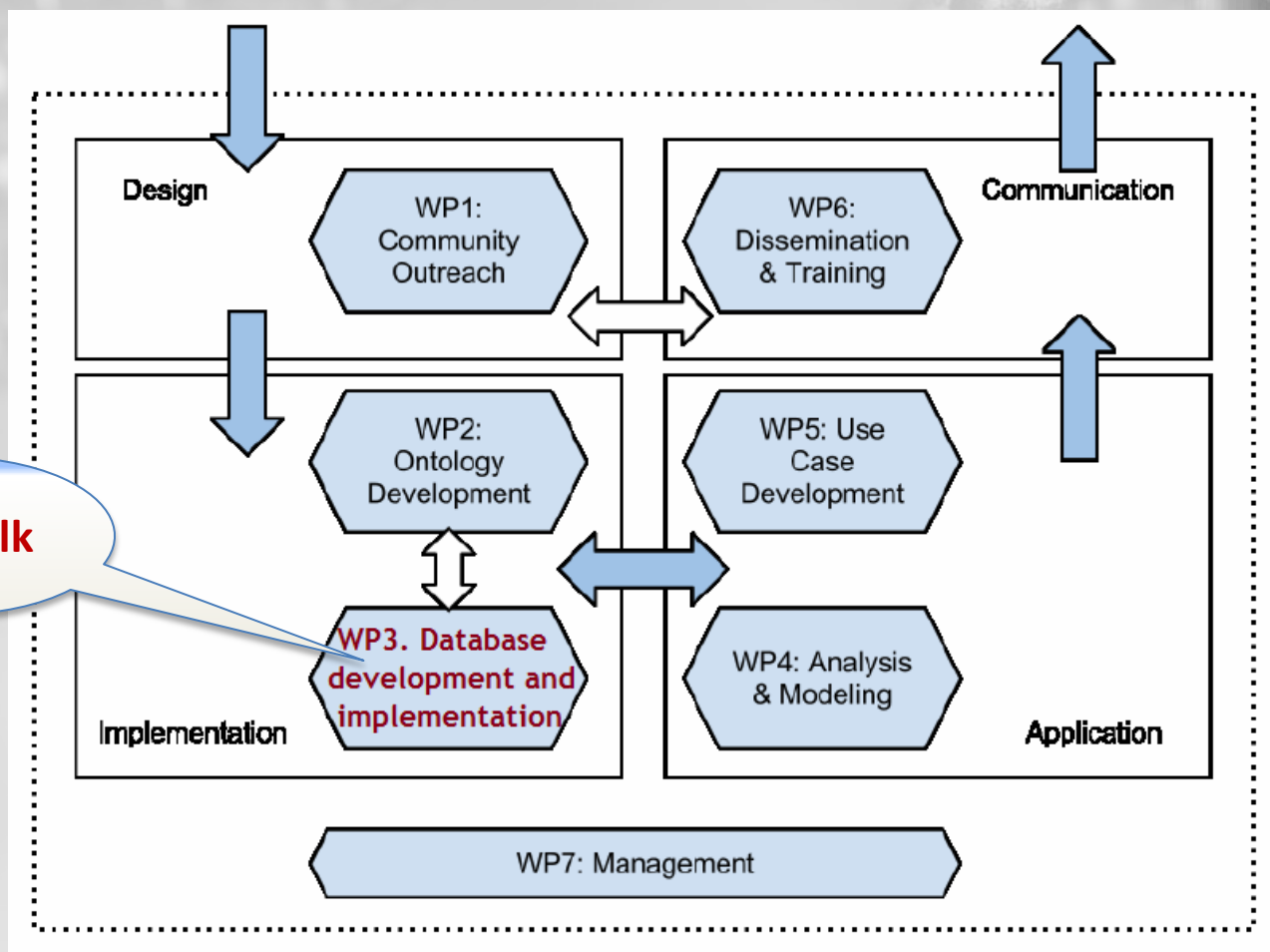


1/29/2015

Our vision

- (re)use open ontologies
 - CHEMINF, NPO, BAO, QUDT
- Based on OpenTox API
 - EU FP7 projects: OpenTox ToxBank
 - Open Source implementations (incl. ambit.sf.net)
- Application Programming Interfaces (APIs)
 - Allow bridging with data analysis tools
 - Exchange formats (ISA-TAB, RDF, ...)

Work packages



This talk

eNanomapper DB review (Q1 2014)

- 104 potential data sources.
- A subset of 34 were publicly available online on the Internet.
- Most of these sources don't provide machine readable data
- Simple web pages : 18
- PDF documents : 10
- Excel tables : 3

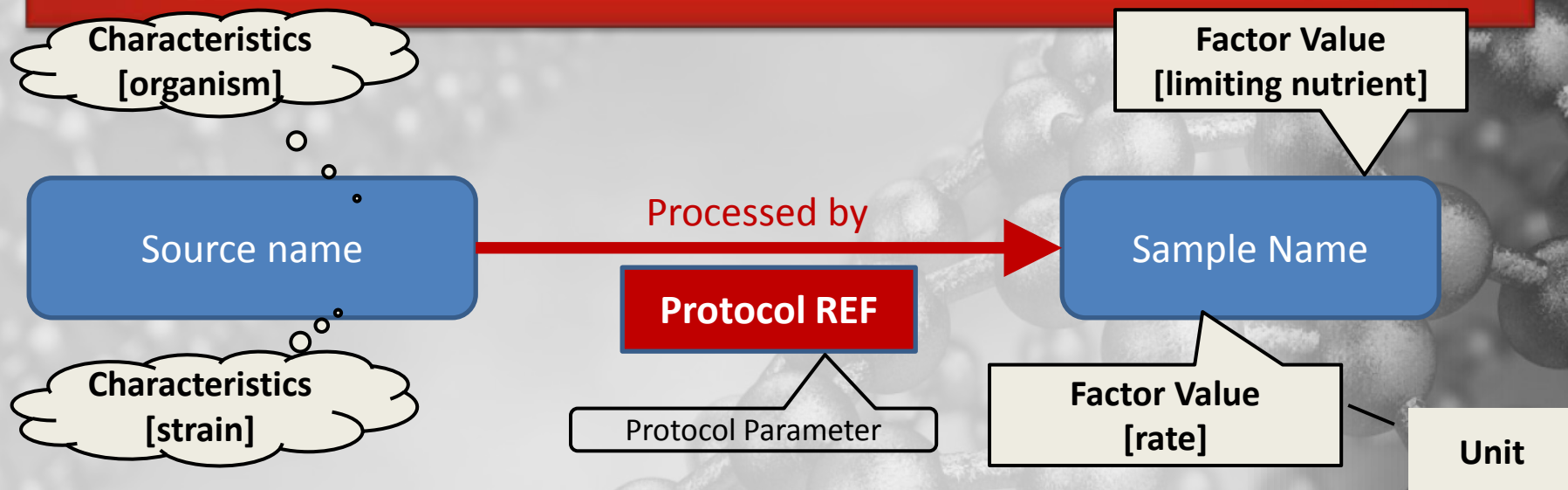
Contributed ~30 entries to the Spring 2014 NSC Database Survey

- Database dumps : 3
- ISA-Tab-Nano format : 1
- IUCLID5 format : 1
- Semantic MediaWiki : 1
- Programmatic access through a publicly available API : 4
- Only one source makes distinction between raw and processed data and provides access to both types of data.



Nanomaterials representation

- **Nanomaterials**
 - Core
 - Coating(s)
 - Linkage
 - Impurities
 - Components, internal structure, etc.
- **Typical assay description**
 - Property – value (range of values) – units (*Excel templates*)
- **More complex description:**
 - Experimental graph (*ISA-TAB / ISA-TAB-nano*)
- **Existing data models**
 - *BioAssay Ontology*
 - *OECD Harmonized Templates*
 - *CoDATA UDS*
 - *ISA-TAB- Nano*
- **Commonalities:**
 - Materials sample
 - Protocols, protocol parameters
 - Experimental conditions
 - Readouts
 - Measurements,
 - Measurement groups,
 - Raw data, derived data



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

ISA-TAB-Nano

ISA-TAB-NANO 1.2 RELEASE NOTES

Modified the ISA-TAB-Nano 1.1 version to address user comments.

- Removed the Material Linkage column from the **Material File**. The Material Constituent column identifies the materials that are linked if the Material Linkage Type is specified.
- Modified the Material Linkage Type description to indicate that if the linkage type is an entrapment or encapsulation, the Material Type column can specify whether the constituent is entrapped or encapsulated.
- Rephrased **Material File** instructions as follows: "*Materials of different chemical composition or physical characteristics should be described in separate **Material files**.*"
- Enhanced the definition of material Characteristics to indicate that **nominal particle characteristics** (or vendor supplied) should be included in the **Material File** as characteristics. **Experimentally determined characteristics** should be included in the **Assay File**.

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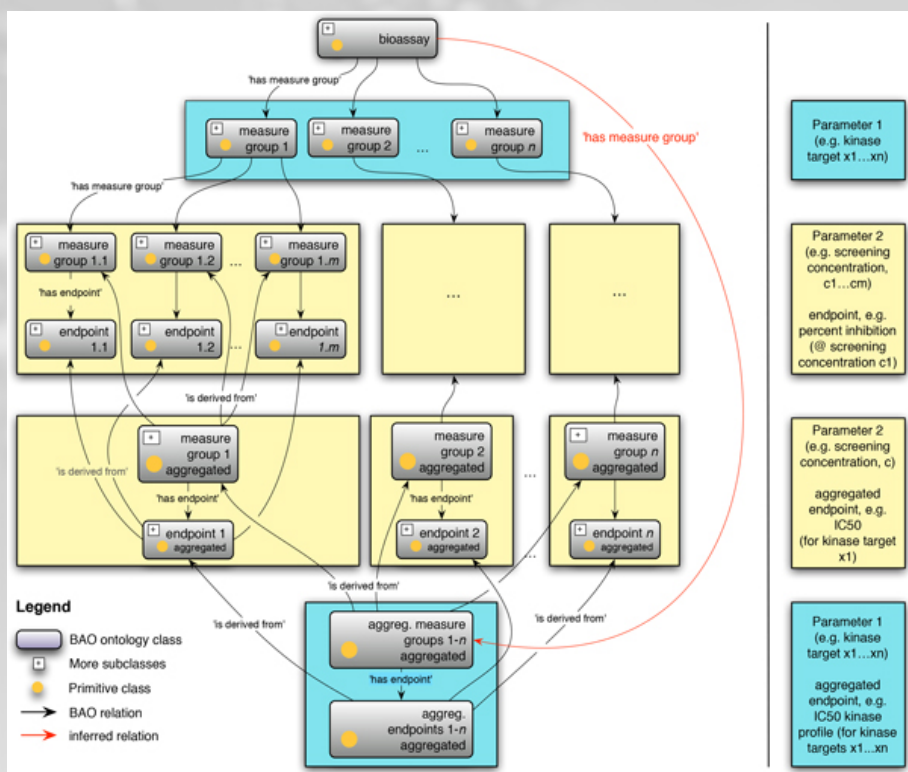
[illegible]

	Q	R	S	T	U
ix Terms	Source	Image	File	Raw Data	Derived D-Comment
var10					
var10					
var10					

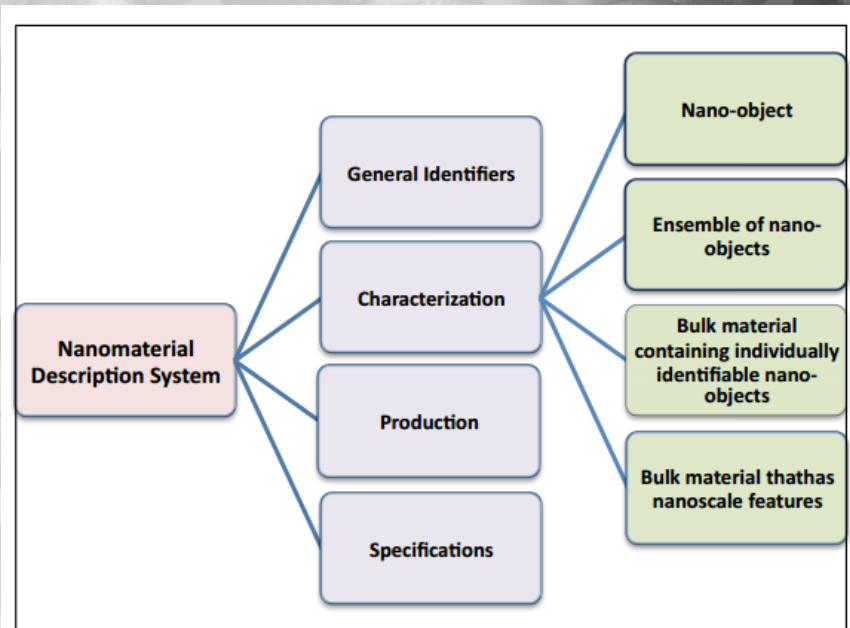
```
G      H
Flat Term Accession Number
#R0 http://purl.bioontology.org/ontology/spot
#R1 http://purl.bioontology.org/ontology/spot
#R2 http://purl.bioontology.org/ontology/spot
#R3 http://purl.bioontology.org/ontology/spot
#R4 http://purl.bioontology.org/ontology/spot
#R5 http://www.imgt.org/download/IMGT-ON
her http://purl.bioontology.org/ontology/CSF/
ing http://purl.bioontology.org/ontology/spot
```

Existing data models (cont)

BioAssay Ontology



CODATA Uniform Description System for Materials at the Nanoscale



Experimental data

- **NPO**

- distinguishes between endpoint of measurement and assay used to measure the endpoint, where the details of the assay could be specified

- **DOI: 10.1007/s11051-013-1455-2**

- “test” and “measurement” terms

- **CODATA UDS**

- requires specification of how particular property is measured.

- **ISA-TAB-Nano**

- allows defining the qualities measured and detailed protocol conditions and instruments.

- **The OECD guideline**

- defines the “test” or “test method” as the experimental system used to obtain the information about a substance. The term “assay” is considered a synonym. The term “Testing” is defined as applying the test method.
- **The endpoints recommended for testing of nanomaterials by OECD WPMN use the terms and categories from the OECD Harmonized Templates.**

- **Summary**

- Specify how a property is measured
- The level of details in the OECD HT, CODATA-UDS, ISA-TAB-Nano and available ontologies differ, which is due to their original focus.

Existing data models: OECD Harmonized Templates

Navigation: Query results, Folders, Section tree

Endpoint study record: Agglomeration/aggregation.001

Detail level: all fields

Administrative Data: Results and discussions, Overall remarks, attachments

Results and discussions

Agglomerate/Aggregate diameter

Mean diameter: 33, St. Deviation: 5, pH: 5, Medium: xxx, Remarks:

Agglomerate/Aggregate size

Percentile D50: 33, Mean: 33, St. Deviation: 5, pH: , Medium: , Remarks:

Agglomerate/Aggregate size distribution at different passages

Seq. Num: , Size: , Distribution: , Remarks:

Agglomeration/Aggregation Index

Mean: , pH: , Medium: , Remarks:

Overall remarks, attachments

Remarks on results incl. tables and figures

4.24 Agglomeration/aggregation

- 4.24.1 Agglomeration/aggregation.001
- 4.25 Crystalline phase
- 4.26 Crystallite and grain size
- 4.27 Aspect ratio/shape
- 4.28 Specific surface area
- 4.29 Zeta potential
- 4.30 Surface chemistry
- 4.31 Dustiness
- 4.32 Porosity
- 4.33 Pour density
- 4.34 Photocatalytic activity
- 4.35 Radical formation potential
- 4.36 Catalytic activity

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Chemical /Toxicogenomics DB (no explicit NM support)



NM: Carbon nanotube assays
>200 fullerenes; metal oxides; silver nanoparticles;
colloidal gold nanoparticles, etc.

ChEMBL



NM: Fullerenes , Metal oxides



Gene expression data
NM: carbon nanotubes, quantum dots, graphene
oxide, zinc oxide, silver and gold nanoparticles.



Comparative Toxicogenomics Database
Includes nanomaterial related data.



The ECHA Dissemination site. Registered chemical
substances under REACH, including NM.



Q: Why no common DB approach?

- Elucidating the data model is difficult
- Making the data model universal is difficult
- Reasons:
 - Material
 - Uniqueness
 - Experimental data
 - Complexity
 - Modelling
 - Different requirements

Analogy: Chemical structures DB

- Chemical structure and properties
- Inappropriate data model.
Instead:
 - **Substances** - **measured properties**
 - Structures - calculated properties.
- Substances composition
 - Constituents, impurities, additives
- Nanomaterials
 - Core, coating(s), linkage
 - Composition
 - Also impurities

What is a “Substance”

- **NPO:**
 - a Nanomaterial (NPO_199) is an equivalent class to chemical substance (NPO_1973)
 - one of (nano-object, nanoparticle, engineered nanomaterial, nanostructured material, nanoparticle formulation).
 - the chemical substance itself is a subclass of a chemical entity (NPO_1972).
- **DOI: 10.1007/s11051-013-1455-2 , . J. Nanoparticle Res. 2013, 15**
 - Compares the definition of the terms “substance” and “material” are in ISO, REACH and general science definitions of the terms. The paper notes the OECD HT definition of “reference substances” is very similar to the definition of the term “reference material”.
- **REACH:** http://echa.europa.eu/documents/10162/13643/nutshell_guidance_substance_en.pdf
 - “Chemical substance, a material with a definite chemical composition”
 - The definition of a substance encompasses all forms of substances and materials on the market, including nanomaterials; and may have complex composition.

Substance (formaldehyde)

formaldehyde

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European Chemical Agency Registration dossier

> Home page

General Information

> Identification

> Compositions

> Aqueous formaldehyde solution (30 % - 60 % formaldehyde)

> Formaldehyde in water

> Aqueous formaldehyde solution (30-58% formaldehyde)

> Formaldehyde

> Aqueous formaldehyde solution (30 % - 60 % formaldehyde)

> Formaldehyde in water

> Aqueous formaldehyde solution (30-58 % formaldehyde)

> Formaldehyde

> Formaldehyde 30% - 60%

> Formaldehyde

> Formaldehyde in water

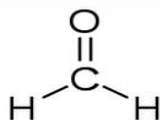
> Aqueous formaldehyde solution (30%-60% formaldehyde)

> Aqueous formaldehyde solution (30 % - 60 % formaldehyde)

> Aqueous formaldehyde solution (30 - 60 % formaldehyde)

Molecular formula CH₂O

IUPAC Name formaldehyde



Constituent

Impurities

methanol

EC Number 200-659-6

EC Name methanol

CAS Number 67-56-1

Molecular formula CH₄O

IUPAC Name methanol

OH

Impurity

Compositions

Substance (25155-25-3)

[1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[tert-butyl] peroxide

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European Chemical Agency Registration dossier

Home page

General Information

Identification

Compositions

Peroxide, 1,1'-[1,3 (or 1,4)-phenylenebis(1-methylethylidene)]bis[2-(1,1d-dimethylethyl)]

[1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[tert-butyl] peroxide

Reaction mass of 1,3-bis[2-(terbutylperoxy)propan-2-yl]benzene and 1,4-bis[2-(terbutylperoxy)propan-2-yl]benzene

Classification and Labelling

Manufacture, Use & Exposure

PBT assessment

Identification

Substance identification

[1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[tert-butyl] peroxide

EC Number 246-678-3

EC Name [1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[tert-butyl] peroxide

CAS Number 25155-25-3

Molecular formula C₂₀H₃₄O₄

IUPAC Name Reaction mass of 1,3-bis[2-(terbutylperoxy)propan-2-yl]benzene and 1,4-bis[2-(terbutylperoxy)propan-2-yl]benzene

Type of substance

Composition multi constituent substance

Origin organic

Trade names

Perkadox 14

Perkadox 14-40

Reaction mass of ...

Multi constituent substance

Substance (formaldehyde)

- 1 -

<

Constituent

Impurity

Additive

Gold nanoparticle

Search ▾

Nanomaterials ▾

OpenTox ▾

Demo ▾

Help ▾

Search substances by identifiers

Showing from 1 to 1 in pages of 10 substances

Previous

Next

Filter...

	Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info	
<div>- 1 -</div>	G15.AC	FCSV-bc77c03d-4...	nanoparticle	G15.AC	FCSV-50cca421-d...	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Anionic	
<div>Composition name:</div> <div>Composition UUID: FCSV-bc77c03d-4e75-3fab-bb3d-17b983663819</div> <div>Purity of IUC Substance:</div>								
	Type	Name	EC No.	CAS No.	Typical concentration	Concentration ranges		Structure
Core		[Au]			0 % (w/w)	0 % (w/w)	0 % (w/w)	Also contained in... <div>Au</div>
Coating		(2 <i>r</i>)-2-Acetamido-3-Sulfanyl-Propanoic Acid, Pwkskimoespyia-Bypyzuensa-N, Inchi=1s/C5h9no3s/C1-3(7)6-4(2-10)5(8)9/H4,10h,2h2,1h3,(H,6,7)(H,8,9)T4-/M0/S1,(2 <i>r</i>)-2-Acetamido-3-Sulfanylpropanoic Acid,(2 <i>r</i>)-2-Acetamido-3-Mercapto-Propionic Acid,(2 <i>r</i>)-2-Acetamido-3-Mercaptopropanoic Acid,N-Acetyl-L-Cysteine			0 % (w/w)	0 % (w/w)	0 % (w/w)	Also contained in...

Core

Coating

Core

Coating

What we need to describe NM and related experiments

What we need to describe a nanomaterial and related experiments

- **A.** An ontology describing a material and the manner of the manufacture (i.e., a single nanoparticle could be a set of ontology annotations, rather than an unique one. A is used to annotate samples of nanomaterials of the same type. Could also relate to an unique naming of a NM as defined by [NanoDefine](#) and [FUTURENANO NEEDS](#) project.
- **B.** Sample level specific to the experiment - defined in *m_*.file* ISA-TAB-nano
- **B.1.** - be able to define composition of the sample. It will typically be composed of several entities (e.g. particle nucleus + coating = multiple rows in ISA-TAB-nano *m_*.file*). It may eventually have different compositions (similar to substances in [LIFE](#)).
- **B.2.** The composition will be linked to chemical structures where relevant (e.g. silver nanoparticle - linked to Ag - as in [OpenChemicals API](#))

- **C.** Attach measurements to **B**. A *measurement* is defined by applying a protocol **P** (with certain parameters) to the sample **B**. The experimental design might include several sets of conditions/factors (e.g. species, concentrations, etc.) and one or more readouts (results). The parameters, conditions are specific for given technology and endpoint measured and defined by minimum information standards.

- **C.1.** Protocol parameters
- **C.2.** Experiment conditions
- **C.3.** Experiment readouts/results
- **C.4.** Reliability
- **D.** Experimental data - good or bad? process or product? (use the Biological Ontology "Measurement" Group Concept)

Unique identifier
Substance / Material
(composition, linkage)

Measurements
(Protocol, parameters,
raw data, derived data)

eNanoMapper prototype database



Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

[nina] Log out

Welcome to eNanoMapper prototype database

A substance database to support safe-by-design engineered nano materials

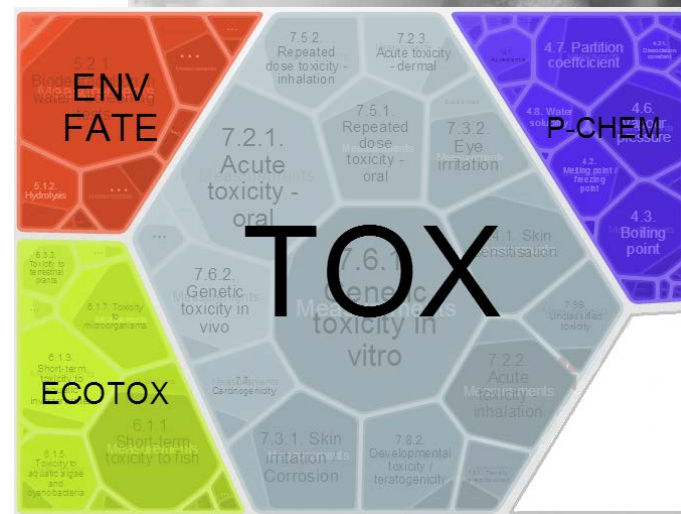
Simple search

Enter chemical name, identifiers, SMILES, InChI

[Au]

Search

Advanced: [Structure search](#) | [Search nanomaterials by identifiers](#) | [Search nanomaterials by endpoint data](#)





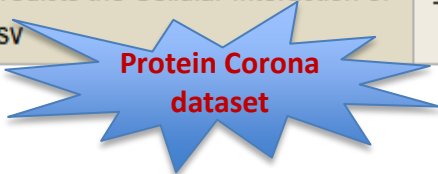
REST API documentation:
<http://enanomapper.github.io/API/>



Nanomaterials overview

[Search ▼](#)[Nanomaterials ▼](#)[OpenTox ▼](#)[Demo ▼](#)[Help ▼](#)[Home](#) > [Admin](#) > [Statistics](#) > [Substances per owner](#)

Showing 1 to 4 of 4 entries

Substance contributor Name ▲	Substances ◇	Table view ◇	
Ideaconsult Ltd. / Sofia / Bulgaria 	Substances [1]	Substances and data Chemical structures	IUC5-354430
NanoWiki 	Substances [330]	Substances and data Chemical structures	NWKI-9F4E8
OECD / Paris / France	Substances [1]	Substances and data Chemical structures	IUC4-44BF02
Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv 	Substances [121]	Substances and data Chemical structures	FCSV-31961

Show

10 ▼

entries



Multi-Walled Carbon Nanotubes

Multi-Walled Carbon Nanotubes (MWCNT), synthetic graphite in tubular shape

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> Home page

■ General Information

> Identification

> Compositions

■ Classification and Labelling

■ Manufacture, Use & Exposure

■ Physical and chemical properties

> Appearance/physical state/colour

> Melting point/freezing point

> Boiling point

> Density

> Particle size distribution (Granulometry)

> Vapour pressure

> Partition coefficient

> Water solubility

> Surface tension

> Flash point

> Auto flammability

> Flammability

> Explosiveness

> Oxidising properties

> Stability in organic solvents and identity of relevant degradation



Search ▾

Nanomaterials ▾

OpenTox ▾

Demo ▾

Help ▾

🏠 > Substance > IUC5-5f313d1f-4129-499c-abbe-ac18642e2471 > Study

IUC Substance Composition P-Chem (5) Tox (3)

Filter...

Expand all Collapse all

Multi-Walled Carbon Nanotubes (MWCNT), Synthetic Graphite In Tubular Shape

7.2.1 Acute toxicity - oral (1)

Species	Endpoint	Value	Sex	Interpretation of the results	Guideline	Study year	Owner	UUID
rat	LDLo	>= 2000	female	practically nontoxic	OECD Guideline 423 (Acute Oral toxicity - Acute Toxic Class Method)	2006		IUC5-49179f2f-867c-4e7c-8f...
	LD50 cut-off	>= 5000	female					

Showing 1 study(s) (1 to 1)

◀ Previous Next ▶

7.6.1 Genetic toxicity in vitro (1)


Genotoxicity type	Study type	Meta-activ. syst.	Target gene	Species/strain	Metabolic activation	Genotoxicity	Interpretation of the result	Guideline	Study year	Owner	UUID
chromosome and DNA damage	Micronucleus test in vitro (MNvit) and Comet assay in vitro	-	-	A549	without	negative	-		2011		IUC5-6bdaad41-66c2-...
				A549	without	negative					

Showing 1 study(s) (1 to 1)

◀ Previous Next ▶

7.7 Carcinogenicity (1)

MWCNT (Phys-chem)


Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

[Home](#) > [Substance](#) > IUC5-5f313d1f-4129-499c-abbe-ac18642e2471 > [Study](#)

IUC Substance Composition P-Chem (5) Tox (3)

Expand all Collapse all

Multi-Walled Carbon Nanotubes (MWCNT), Synthetic Graphite In Tubular Shape

4.1 Appearance (1)

Physical state	Remark	Substance type	Guideline	Owner	UUID
solid	nanomaterial	inorganic			IUC5-9db5f020-e0fa-47c8-8...

Showing 1 study(s) (1 to 1)

[Previous](#) [Next](#)

4.5 Particle size distribution (Granulometry) (1)

Test Material Form	Dist. type num.	Endpoint	Value	Std. dev.	Reference	Guideline	Owner	UUID
-	imaging	MASS MEDIAN DIAMETER	[3, 20]	-	2011	Transmission Electron Microscopy (TEM)		IUC5-4bca14fc-3e43-435e-...
	tec	MASS MEDIAN AERODYNAMIC DIAMETER		-				
	hnique	PARTICLE SIZE.D90	= 12.7	-				

Showing 1 study(s) (1 to 1)

[Previous](#) [Next](#)

4.28 Nanomaterial specific surface area (1)

4.29 Nanomaterial zeta potential (1)

Type of method	Test Material Form	Endpoint	Result	Remarks	Std. dev.	pH	Medium	Reference	Guideline	Owner	UUID
-	-	ZETA POTENTIAL	= 41.4	-	= 2.9	= 1.9	-	2010			IUC5-708684e4-4e3b-49cd-...
		ZETA POTENTIAL	= 39.3	-	= 1.5	= 2.99	-				
		ZETA POTENTIAL	= 21.4	-	= 6.5	= 4.26	-				
		ZETA POTENTIAL	= 34.5	-	= 1.7	= 5.04	-				

Showing 1 study(s) (1 to 1)

[Previous](#) [Next](#)

4.31 Nanomaterial dustiness (1)

Prototype database (Protein Corona)

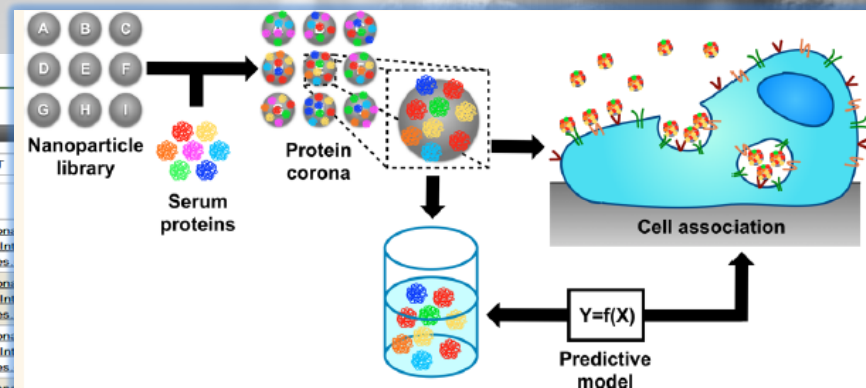
ENM eNanoMapper

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	ECSV-2a853f39-4...	nanoparticle	G15.DDT@BDHDA	ECSV-2a853f39-4...	Protein Corona the Cellular Int...
- 12 -	G15.DDT@CTAB	ECSV-d1731b11-2...	nanoparticle	G15.DDT@CTAB	ECSV-d1731b11-2...	Protein Corona the Cellular Int...
- 13 -	G15.DDT@DOTAP	ECSV-3b96ad7a-b...	nanoparticle	G15.DDT@DOTAP	ECSV-3b96ad7a-b...	Protein Corona the Cellular Int...
- 14 -	G15.DDT@ODA	ECSV-fb5e6048-8...	nanoparticle	G15.DDT@ODA	ECSV-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	Also contained	Structure
Coating	Dodecane-1-Thiol, Wnahlmidsqwp-Uhfflaoya-N, Inch=1s/C 12h26u/C 1-2-3-4-5-6-7-8-9-10-11-12-13h11h.2-12h2, 1h3, 1-Dodecanethiol			0 % (w/w)	0 % (w/w)	Also contained	
Coating	Octadecan-1-Amine, Rxyjpsvyrzge-Uhfflaoya-N, Inch=1s/C 18h39u/C 1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19h12-10h2, 1h3, Stearylamine, 1-Octadecanamine, Octadecylamine			0 % (w/w)	0 % (w/w)	Also contained	
Core	[Au]			0 % (w/w)	0 % (w/w)	Also contained	Au

Search:

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

Prototype database (Protein Corona)

Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

Home > Substance > FCSV-fb5e6048-8ee1-351d-915b-d1669681357e > Study

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

Filter...

Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

Home > Substance > FCSV-fb5e6048-8ee1-351d-915b-d1669681357e > Study

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

Filter...

Expand all Collapse all

G15.DDT@ODA

7.100 Proteomics (1)

7.99 Unclassified toxicity (4)

DATA_GATHERER	Type of method	test	MEDIUM	Endpoint	Result	Text	result	Guideline	Owner	UUID
-	Serum.density	-	Human serum (Sigma #H4522)	Total protein (BCA assay)	mean 0.412	-	-	doi: 10.1021/nn406018q	-	FCSV-6e5bbb4f-3c98-3456-...
-	Serum.density	-	Human serum (Sigma #H4522)	Autot (ICP-AES)	mean 257.8317343	-	-	doi: 10.1021/nn406018q	-	FCSV-fc4ce3f1-487a-308b-b...
-	Serum.density	-	Human serum (Sigma #H4522)	Total surface area (SATot)	mean 11	-	-	doi: 10.1021/nn406018q	-	FCSV-fc4ce3f1-487a-308b-b...
-	Serum.density	-	Human serum (Sigma #H4522)	Protein density	-	-	-	doi: 10.1021/nn406018q	-	FCSV-fc4ce3f1-487a-308b-b...
Perkin-Elmer	ICP-AES	-	-	Net cell association	mean 0.01436	-	-	doi: 10.1021/nn406018q	-	FCSV-6f5ba7be-0358-359e-...
-	ICP-AES	-	-	Log2 transformed	mean -6.122	-	-	doi: 10.1021/nn406018q	-	FCSV-6f5ba7be-0358-359e-...
UV-1601PC absorba	Absorbance.sp	-	Human serum (Sigma #H4522)	Localized Surface Plasmon Resonance (LSPR) index	mean 0.309989179	-	-	doi: 10.1021/nn406018q	-	FCSV-10542832-b372-3663-...
nance spectrophot	ectrophotometr	-	Human serum (Sigma #H4522)	Localized Surface Plasmon Resonance (LSPR) index	mean 0.367331174	-	-	doi: 10.1021/nn406018q	-	FCSV-10542832-b372-3663-...
ometer (Shimadzu)	y.AS.	-	Human serum (Sigma #H4522)	LSPR peak position (nm)	mean 521.43	-	-	doi: 10.1021/nn406018q	-	FCSV-10542832-b372-3663-...

Showing 4 study(s) (1 to 4)

Previous Next

Help: Substances
Chemical substance, a material with a definite chemical composition. [REACH guide](#)
Mono-constituent ? and multi-

Prototype database (NanoWiki)

ENM eNanoMapper

Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾ Log

> Search substances by identifiers

Substance search ?

External identifier ▾

Search

Study ? : P-Chem ENV ECO TOX

Reliability ? : 1 2 3 4 5 6

Study purpose ? : K S WoE D N/A




Robust study ? : Yes No

Result ? : E EP C RAQ RAa Q O ND NA

JSON

Help: Substances
Chemical substance, a material with a definite chemical composition. REACH guide C₀
Mono-constituent ? and multi-constituent ?
substances. Main constituent ? Additive ? Impurity ?





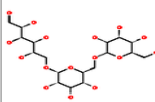

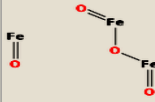
Showing from 1 to 10 in pages of 10 substances Previous Next Filter...

	Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info																			
- 1	Kim2012 NM1	NWKI-71060af4-1...	MetalOxide	CuO	NWKI-71060af4-1...	NanoWiki	Composition = CuO DATASET = NanoWiki Has_Identifier = 139																			
- 2	Zhou2008 M60	NWKI-00e60625-9...	CarbonNanotube	64	NWKI-00e60625-9...	NanoWiki	Composition = C DATASET = NanoWiki Has_Identifier = 292 SOURCE = Zhou2008																			
- 3	Zhou2008 M15	NWKI-f805b6f2-65...	CarbonNanotube	19	NWKI-f805b6f2-65...	NanoWiki	Composition = C DATASET = NanoWiki Has_Identifier = 227 SOURCE = Zhou2008																			
- 4	Zhou2008 M29	NWKI-a40c7554-4...	CarbonNanotube	33	NWKI-a40c7554-4...	NanoWiki	Composition = C DATASET = NanoWiki Has_Identifier = 241 SOURCE = Zhou2008																			
- 5	Zhou2008 M25	NWKI-8ba8821c-f...	CarbonNanotube	29	NWKI-8ba8821c-f...	NanoWiki	Composition = C DATASET = NanoWiki Has_Identifier = 237 SOURCE = Zhou2008																			
- 6	Limbach2005 NM1	NWKI-7998492c-3...	MetalOxide	CeO2 I	NWKI-7998492c-3...	NanoWiki	Composition = CeO2 DATASET = NanoWiki Has_Identifier = 161																			
- 7	Zhang2013 M17	NWKI-c10e9034-a...	MetalOxide	SiO2	NWKI-c10e9034-a...	NanoWiki	Composition = SiO2 DATASET = NanoWiki Has_Identifier = 322 SOURCE = Zhang2012																			
<p>Composition name: Composition UUID: NWKI-c10e9034-a37c-37f8-afa4-b0e1081c6856</p> <table border="1"> <thead> <tr> <th>Type</th> <th>Name</th> <th>EC No.</th> <th>CAS No.</th> <th>Typical concentration</th> <th colspan="3">Concentration ranges</th> <th>Also contained</th> <th>Structure</th> </tr> </thead> <tbody> <tr> <td>Core</td> <td>SiO2</td> <td></td> <td>7631-86-9</td> <td>0 % (w/w)</td> <td>0 % (w/w)</td> <td>0 % (w/w)</td> <td>SiO2</td> <td></td> </tr> </tbody> </table>								Type	Name	EC No.	CAS No.	Typical concentration	Concentration ranges			Also contained	Structure	Core	SiO2		7631-86-9	0 % (w/w)	0 % (w/w)	0 % (w/w)	SiO2	
Type	Name	EC No.	CAS No.	Typical concentration	Concentration ranges			Also contained	Structure																	
Core	SiO2		7631-86-9	0 % (w/w)	0 % (w/w)	0 % (w/w)	SiO2																			
- 8	Zhou2008 M6	NWKI-08b685e5-7...	CarbonNanotube	10	NWKI-08b685e5-7...	NanoWiki	Composition = C DATASET = NanoWiki Has_Identifier = 218 SOURCE = Zhou2008																			
- 9	Lesniak2013 NM1	NWKI-895a506b-c...	PolymerCore	40 nm PS-COOH	NWKI-895a506b-c...	NanoWiki	Composition = C8H8 DATASET = NanoWiki Has_Identifier = 296 SOURCE = Lesniak2013																			
- 10	Antisari2013 M1	NWKI-6d5462cc-7...	MetalOxide	CeO2	NWKI-6d5462cc-7...	NanoWiki	Composition = CeO2 DATASET = NanoWiki Has_Identifier = 300 SOURCE = Antisari2013																			



NanoWiki : literature data
Egon Willighagen
(Karolinska Institutet,
Maastricht University)



NM components (NanoWiki)

<div>  <div> Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾ </div> </div>							
<div>  Search substances by identifiers </div>							
<div>  - 1 - </div>	Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info
	Shaw51 45	NWKI-02981dd4-b...	MetalOxide	MION-47 no. 35	NWKI-02981dd4-b...	NanoWiki	Alternative Identifier = NP45 Coating = DextranCoating Composition = Fe3O4 DATASET = NanoWiki Has_Identifier = 75
Composition name: Composition UUID: NWKI-02981dd4-b7d0-34c8-a0ab-dd19a5a40865							
Type	Name	EC No.	CAS No.	Typical concentration	Concentration ranges		Structure
Coating	 (2r,3s,4r,5r)-6-[(2s,3r,4s,5s,6r)-6-[[[(2s,3r,4s,5s,6r)-6-(Hydroxymethyl)-3,4,5-Tris(Oxidanyl)Oxan-2-Y]]Oxymethyl]-3,4,5-Tris(Oxidanyl)Oxan-2-Y]]Oxy-2,3,4,5-Tetrakis(Oxidanyl)Hexanal,Fzwbhnmjmcdu-Blauphosa-N,Inchi=1s/C18h32o16/C19-1-5(21)9(23)10(24)9(22)3-31-17-16(30)14(28)12(26)8(34-17)4-32-18-15(29)13(27)11(25)7(2-20)33-18/H1,5-18,20-30h,2-4h2/T5-.6+,7+,8+,9+,10+,11+,12+,13-,14-,15+,16+,17-,18-/M0/S1,(2r,3s,4r,5r)-2,3,4,5-Tetrahydroxy-6-[(2s,3r,4s,5s,6r)-3,4,5-Trihydroxy-6-[[[(2s,3r,4s,5s,6r)-3,4,5-Trihydroxy-6-(Hydroxymethyl)Tetrahydropyran-2-Y]]Oxymethyl]Tetrahydropyran-2-Y]]Oxy-Hexanal,(2r,3s,4r,5r)-2,3,4,5-Tetrahydroxy-6-[(2s,3r,4s,5s,6r)-3,4,5-Trihydroxy-6-[[[(2s,3r,4s,5s,6r)-3,4,5-Trihydroxy-6-(Hydroxymethyl)Oxan-2-Y]]Oxymethyl]Oxan-2-Y]]Oxyhexanal,(2r,3s,4r,5r)-2,3,4,5-Tetrahydroxy-6-[(2s,3r,4s,5s,6r)-3,4,5-Trihydroxy-6-[[[(2s,3r,4s,5s,6r)-3,4,5-Trihydroxy-6-Methylol-Tetrahydropyran-2-Y]]Oxymethyl]Tetrahydropyran-2-Y]]Oxy-Hexanal,(2r,3s,4r,5r)-2,3,4,5-Tetrahydroxy-6-[[[(2s,3r,4s,5s,6r)-3,4,5-Trihydroxy, Dextran			0 % (w/w)	0 % (w/w)	0 % (w/w)	Also contained in... 
Core	 Fe3O4		1317-61-9	0 % (w/w)	0 % (w/w)	0 % (w/w)	Also contained in... 

Prototype database: Phys chem & Tox (NanoWiki)



 Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

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

IUC Substance Composition P-Chem (4) Tox (5)

Filter... Expand all Collapse all

Micron

4.5 Particle size distribution (Granulometry) (2)

Test Material Form	Distrib type	Passag num.	Endpoint	Value	Reference	Guideline	Method type	Owner	UUID
-	-	-	PARTICLE SIZE	= 221	DOI	DLS	DLS	-	NWKI-2433959f-8955-48b0-...
-	-	-	PARTICLE SIZE	= 221	DOI		-	-	NWKI-bc3b5b48-5780-401e-...

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

IUC Substance Composition P-Chem (4) Tox (5)


Micron

8.100 Cell Viability Assay (5)

Reference	Cell line	Doses/concentrations	Endpoint	Result	Result (text)	Guideline	Owner	UUID
2011	HaCaT	= 100 mg/L	Percentage Viable Cells	= 95	-		Chemosphere	NWKI-ae63ad42-ee3c-450a-...
http://dx.doi.org/10.1016/j.chemosphere.2011.04.067	HaCaT	= 500 mg/L	Percentage Viable Cells	= 98	-		Chemosphere	NWKI-5c9e9e91-0c88-4faa-...
2011	HaCaT	= 1000 mg/L	Percentage Viable Cells	= 92	-		Chemosphere	NWKI-fb9a42a3-ce97-45fc-...
2011	HaCaT	= 10 mg/L	Percentage Viable Cells	= 101	-		Chemosphere	NWKI-1bcd287a-291e-4173-...
2011	HaCaT	= 7000 mg/L	Percentage Viable Cells	= 74.3	-		Chemosphere	NWKI-72a4393b-5dd7-4bcf-...

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

NM toxicity (classifier)



Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾
Log

[Substance](#) > [NWKI-8ef21404-e101-37c8-8206-32f526d75012](#) > [Study](#)

[Show structures](#)
[Show composition](#)
[Substance search ?](#)

External identifier ▾

[Study ? : P-Chem](#)
[ENV ECO TOX](#)
[Reliability ? : 1 2 3 4 5 6](#)
[Study purpose ? : K S WoE D N/A](#)
[Robust study ? : Yes No](#)
[Result ? : E EP C RAg RAa Q O ND NA](#)
[JSON](#)










[Help: Substances](#)
 Chemical substance, a material with a definite chemical composition. [REACH guide](#) 
 Mono-constituent ? and multi-constituent ? substances. Main constituent ? Additive ?
 Impurity ?

IUC Substance Composition P-Chem (1) **Tox (9)**

Expand all Collapse all

CuO

8.100 Cell Viability Assay (9)

Reference	Cell line	Doses/concentration	Endpoint	Result	Result (text)	Guideline	Owner	UUID
2011	BEAS-2B	= 1 mg/L	Toxicity Classifier		Non-toxic		Small	NWKI-64c2f9f2-15fc-4406-a 
2011 http://dx.doi.org/10.1002/sml.201002366	BEAS-2B	= 10 mg/L	Toxicity Classifier		Non-toxic		Small	NWKI-e0ba8151-b48f-4509- 
2011	BEAS-2B	= 100 mg/L	Toxicity Classifier		Non-toxic		Small	NWKI-4eb1d350-4989-4f22- 
2011	BEAS-2B	= 150 mg/L	Toxicity Classifier		Toxic		Small	NWKI-8ac45587-5aaa-44bb- 
2011	BEAS-2B	= 20 mg/L	Toxicity Classifier		Non-toxic		Small	NWKI-d98d2503-ab99-4cf0- 
2011	BEAS-2B	= 200 mg/L	Toxicity Classifier		Toxic		Small	NWKI-30aedbfd-11e3-4f2f-b 
2011	BEAS-2B	= 25 mg/L	Toxicity Classifier		Non-toxic		Small	NWKI-fa792b70-953a-4bad- 
2011	BEAS-2B	= 5 mg/L	Toxicity Classifier		Non-toxic		Small	NWKI-5875076e-c37c-462c- 
2011	BEAS-2B	= 50 mg/L	Toxicity Classifier		Non-toxic		Small	NWKI-cf171f6d-3bd9-44bd- 

Showing 9 study(s) (1 to 9)
 ◀ Previous Next ▶

NM toxicity (numeric)



Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

Log

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

Show structures

Show composition

Substance search ?

External identifier ▾

Search

Study ? : P-Chem
ENV ECO TOX

Reliability ? : 1 2 3 4
5 6

Study purpose ? : K S
WoE D N/A

Robust study ? : Yes
No

Result ? : E EP C RAQ
RAA Q Q ND NA

JSON

Help: Substances

IUC Substance Composition P-Chem (4) Tox (5)

Filter...

Expand all Collapse all

Micron

8.100 Cell Viability Assay (5)

Reference	Cell line	Doses/concentrations	Endpoint	Result	Result (text)	Guideline	Owner	UUID
2011	HaCaT	= 10 mg/L	Percentage Viable Cells	= 101	-		Chemosphere	NWKI-1bcd287a-291e-4173-...
2011	HaCaT	= 500 mg/L	Percentage Viable Cells	= 98	-		Chemosphere	NWKI-5c9e9e91-0c88-4faa-...
2011	HaCaT	= 7000 mg/L	Percentage Viable Cells	= 74.3	-		Chemosphere	NWKI-72a4393b-5dd7-4bcf-...
2011	HaCaT	= 100 mg/L	Percentage Viable Cells	= 95	-		Chemosphere	NWKI-ae63ad42-ee3c-450a-...
2011	HaCaT	= 1000 mg/L	Percentage Viable Cells	= 92	-		Chemosphere	NWKI-fb9a42a3-ce97-45fc-...

Showing 5 study(s) (1 to 5)

Previous Next



Search by particle size

Search substances by endpoint data ▾ Hit list

Showing from 31 to 40 in pages of 10 substances ▾ Previous ▾ Next ▾

Filter...

Update results

▼ P-Chem

- ☐ 4.1. Appearance (S) [3]
- ☐ 4.2. Melting point / freezing point (S) [3]
- ☐ 4.26. Nanomaterial crystallite and grain size (S) [105]
- ☐ 4.27. Nanomaterial aspect ratio/shape (S) [3]
- ☐ 4.28. Nanomaterial specific surface area (S) [8]
- ☐ 4.29. Nanomaterial zeta potential (S) [248]
- ☐ 4.3. Boiling point (S) [5]
- ☐ 4.30. Nanomaterial surface chemistry (S) [367]
- ☐ 4.31. Nanomaterial dustiness (S) [1]
- ☒ 4.5. Particle size distribution (Granulometry) (S) [496]
- ☐ 4.6. Vapor pressure (S) [1]
- ☐ 4.7. Partition coefficient (S) [3]
- ☐ 4.8. Water solubility (S) [4]

Endpoint name: Units:

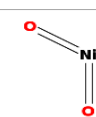

Value:

Env Fate

Eco Tox

Tox

Update results

	Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info
- 31 -	Cytotox2011Puzyn16	NWKI-3b09fdd1-3...	MetalOxide	Cr2O3	NWKI-3b09fdd1-3...	NanoWiki	Composition = Cr2O3 DATASET = NanoWiki Has_Identifier = 16
- 32 -	Cytotox2011Puzyn10	NWKI-a9ef3839-f1...	MetalOxide	SiO2	NWKI-a9ef3839-f1...	NanoWiki	Composition = SiO2 DATASET = NanoWiki Has_Identifier = 10
- 33 -	Cytotox2011Puzyn05	NWKI-3e42f6e5-6...	MetalOxide	Bi2O3	NWKI-3e42f6e5-6...	NanoWiki	Composition = Bi2O3 DATASET = NanoWiki Has_Identifier = 6
- 34 -	Cytotox2011Puzyn15	NWKI-905e44ef-3f...	MetalOxide	NiO	NWKI-905e44ef-3f...	NanoWiki	Composition = NiO2 DATASET = NanoWiki Has_Identifier = 15
Composition UUID: NWKI-905e44ef-3f7f-314d-add0-3e00439eadd							
Type	Name	EC No.	CAS No.	Typical concentration	Concentration ranges		Structure
Core	NiO2			0 % (w/w)	0 % (w/w)	0 % (w/w)	Also contained in... 
- 35 -	Gopalan2009 NM2	NWKI-dd6b8324-5...	MetalOxide	TiO2	NWKI-dd6b8324-5...	NanoWiki	Composition = TiO2 DATASET = NanoWiki Has_Identifier = 160
- 36 -	Cytotox2011Puzyn01	NWKI-e2aed1b9-f...	MetalOxide	ZnO	NWKI-e2aed1b9-f...	NanoWiki	Composition = ZnO DATASET = NanoWiki Has_Identifier = 2
Composition UUID: NWKI-e2aed1b9-f918-3000-934c-0e13b7d5c977							
Type	Name	EC No.	CAS No.	Typical concentration	Concentration ranges		Structure
Core	ZnO	215-222-5	1314-13-2	0 % (w/w)	0 % (w/w)	0 % (w/w)	Also contained in... 
- 37 -	Cytotox2011Puzyn04	NWKI-ca37d03d-a...	MetalOxide	Y2O3	NWKI-ca37d03d-a...	NanoWiki	Composition = Y2O3 DATASET = NanoWiki Has_Identifier = 5

Endpoint search (tox & pchem)

ENM eNanoMapper

Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾ [Log in](#)

Update results

► P-Chem

► Env Fate

► Eco Tox

▼ Tox

- ☐ 7.100. Proteomics (S) [121]
- ☐ 7.2.1. Acute toxicity - oral (S) [6]
- ☐ 7.2.2. Acute toxicity - inhalation (S) [14]
- ☐ 7.2.3. Acute toxicity - dermal (S) [1]
- ☐ 7.3.1. Skin irritation / Corrosion (S) [2]
- ☐ 7.3.2. Eye irritation (S) [1]
- ☐ 7.4.1. Skin sensitisation (S) [52]
- ☐ 7.5.1. Repeated dose toxicity - oral (S) [8]
- ☐ 7.5.2. Repeated dose toxicity - inhalation (S) [44]
- ☐ 7.5.3. Repeated dose toxicity - dermal (S) [3]
- ☐ 7.6.1. Genetic toxicity in vitro (S) [191]
- ☐ 7.6.2. Genetic toxicity in vivo (S) [67]
- ☐ 7.7. Carcinogenicity (S) [28]
- ☐ 7.8.1. Toxicity to reproduction (S) [6]
- ☐ 7.8.2. Developmental toxicity / teratogenicity (S) [14]
- ☐ 7.99. Unclassified toxicity (S) [469]
- ☒ 8.100. Cell Viability Assay (S) [144]

Endpoint name **Units**

Percentage Viable Cells

Enter endpoint value

>= 90 <=

Result (text)

Update results

Search substances by endpoint data [Hit list](#)

Showing from 1 to 4 in pages of 10 substances [Previous](#) [Next](#) Filter...

	Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info
- 1 -	Field2011 Micron	NWKI-9f37da26-8...	MetalOxide	Micron	NWKI-9f37da26-8...	NanoWiki	Composition = HfO2 DATASET = NanoWiki Has_Identifier = 109
- 2 -	Field2011 Batch2	NWKI-0a6e319e-7...	MetalOxide	Batch 2	NWKI-0a6e319e-7...	NanoWiki	Composition = HfO2 DATASET = NanoWiki Has_Identifier = 107
- 3 -	Field2011 Batch3	NWKI-d8f70c6c-3...	MetalOxide	Batch 3	NWKI-d8f70c6c-3...	NanoWiki	Composition = HfO2 DATASET = NanoWiki Has_Identifier = 108
- 4 -	Field2011 Batch1	NWKI-c4c91023-5...	MetalOxide	Batch 1	NWKI-c4c91023-5...	NanoWiki	Composition = HfO2 DATASET = NanoWiki Has_Identifier = 106

Composition name:
Composition UUID: NWKI-c4c91023-5b41-3d6d-bb4f-ee1152926be0
Purity of IUC Substance:

Type	Name	EC No.	CAS No.	Typical concentration	Concentration ranges	Structure
Core	HfO2		12055-23-1	0 % (w/w)	0 % (w/w) 0 % (w/w)	Also contained in...

Search:

Chemical structure: O=[Hf]=O

Chemical similarity search

ENM eNanoMapper

Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

Search structures and associated data

Exact structure Similarity Substructure URL 0.5 NCCCCC

Diagram

Showing from 1 to 3 in pages of 20 entries Previous Next

Identifiers	Substances	Datasets								
CasRN	EC number	IUCLID 5 R	Names	Trade Name	IUPAC name	SMILES	Std. InChI key	Std. InChI	REACH registration date	Similarity
- 1 -	G60.ODA	FCSV-7a--	nanoparticle	G60.ODA	FCSV-50--	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic	coating		
- 2 -	G15.ODA	FCSV-92--	nanoparticle	G15.ODA	FCSV-50--	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic	coating		
- 3 -	G15.DDT@ODA	FCSV-fbS--	nanoparticle	G15.DDT@ODA	FCSV-50--	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic	coating		

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

Identifiers	Substances	Datasets								
CasRN	EC number	IUCLID 5 R	Names	Trade Name	IUPAC name	SMILES	Std. InChI key	Std. InChI	REACH registration date	Similarity
- 1 -	S40.HDA	FCSV-9e--	nanoparticle	S40.HDA	FCSV-5a--	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic	coating		
- 2 -	G60.HDA	FCSV-as--	nanoparticle	G60.HDA	FCSV-50--	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic	coating		
- 3 -	G15.HDA	FCSV-cdf--	nanoparticle	G15.HDA	FCSV-50--	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic	coating		
- 4 -	G30.DDT@HDA	FCSV-ch--	nanoparticle	G30.DDT@HDA	FCSV-50--	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic	coating		

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

Identifiers	Substances	Datasets								
CasRN	EC number	IUCLID 5 R	Names	Trade Name	IUPAC name	SMILES	Std. InChI key	Std. InChI	REACH registration date	Similarity
- 1 -	G15.AHT	FCSV-8fS--	nanoparticle	G15.AHT	FCSV-50--	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic	coating		

Select data sources/models

Chemical structure diagram showing a molecule with an amine group (H₂N) and a methyl group (CH₃).

Chemical similarity search (MES coating)

ENM eNanoMapper

Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

Search structures and associated data

Exact structure Similarity Substructure URL 0.5 C(CS)CS

Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

Search structures and associated data

Exact structure Similarity Substructure URL 0.5 C(CS)CS(=O)(=O)[O-]

Identifiers Datasets

Showing from 1 to 2 in pages of 20 entries Previous Next

Diagram CAS EINECS IUCLID UUID Name Trade Name IUPAC Name SMILES InChI Key InChI REACH Date Similarity

Identifiers	Substances	Datasets
Substance Name	Substance UUID	Substance Type
- 1 -	Harper2011 8	NWKI-4f...
- 2 -	Harper2011 9	NWKI-56...

2-Mercaptoethanesulfonate

NanoWiki

Protein Corona dataset

Coating

4.5 Particle size distribution (Granulometry) (1)

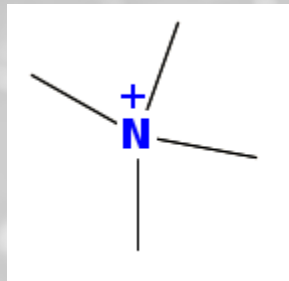
4.30 Nanomaterial surface chemistry (1)

4.5 Particle size distribution (Granulometry) (2)

4.26 Nanomaterial crystallite and grain size (1)

4.29 Nanomaterial zeta potential (1)

Chemical substructure search



Protein Corona
dataset

NanoWiki

ENM eNanoMapper 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

Cationic (quaternary ammonium) surfactants

Diagram CAS EINECS Name Trade Name IUPAC Name SMIL

1 - 2 - 3 - 4 -

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

Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info	Contained in as
Harper2011 6	NWKI-c36...	Metal	Ag	NWKI-c36...	NanoWiki	Coating = TMATCoating Composition = Ag DATASET = NanoWiki Has_Identifier = 96	coating
Harper2011 3	NWKI-e8...	Metal	Ag	NWKI-e8...	NanoWiki	Coating = TMATCoating Composition = Ag DATASET = NanoWiki Has_Identifier = 93	coating
Harper2011 7	NWKI-fe...	Metal	Ag	NWKI-fe...	NanoWiki	Coating = TMATCoating Composition = Ag DATASET = NanoWiki Has_Identifier = 97	coating

Coating

Data upload



Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

Home > Substances > Import > Multiple .isz files upload

Substance search ?

Name ▾

Search

Study ? : P-Chem ENV ECO TOX

Reliability ? : 1 2 3 4 5 6

Study purpose ? : K S WoE D N/A

Robust study ? : Yes No

Result ? : E EP C RAa RAa Q Q ND
NA

JSON

Import new substance(s)

+ Add files...

+ Start upload

○ Cancel upload

Clear existing study records



Clear existing composition records



Import only high quality study records



(uncheck to import all records)

Purpose flag ▴ ▾

key study
supporting study
weight of evidence
disregarded study
Not specified

Study result type ▴ ▾

(Q)SAR
no data
other:
estimated by calculation
experimental result

Test material ▴ ▾

no
yes
Not specified
Not assigned (null)

Reliability ▴ ▾

1 (reliable without restriction)
2 (reliable with restrictions)
3 (not reliable)
4 (not assignable)
other:

Reference type ▴ ▾

other:
publication
review article or handbook
secondary source
study report

▴ Select high quality study criteria

+ Select All

- Unselect all



backup_public_v5.rdf

1.15 MB



IUC4-efdb21bb-e79f-3286-a988-b6f6944d3734.isz

1.78 MB



Protein Corona Fingerprinting Predicts the Cellular
Interaction of Gold and Silver Nanoparticles.csv

414.63 KB

Help: Substances

Chemical substance, a material with a definite chemical composition. [REACH guide](#) [Mono-constituent ?](#) and multi-constituent ? substances. Main constituent ? Additive ? Impurity ?

Under development :


- ISA-TAB-Nano import
- More spreadsheet templates

Substance import options: [Multiple .isz files upload](#) | [Single .isz file upload](#) | [Retrieve substance\(s\) from IUCLID5 server](#)



REST Application Programming Interface

API documentation (Swagger-UI)

ENM  <https://apps.ideaconsult.net/enanomapper/api-docs>

eNanoMapper prototype database API

AMBIT REST web services 2.7.2 (with enanomapper profile). More at <https://apps.ideaconsult.net/enanomapper>
[Terms of service](#)
[Contact the developer](#)
[License](#)

algorithm : OpenTox Algorithms service [Show/Hide](#) [List Operations](#) [Expand Operations](#) [Raw](#)

bundle : Datasets of substances [Show/Hide](#) [List Operations](#) [Expand Operations](#) [Raw](#)

compound : OpenTox Chemical Compounds service [Show/Hide](#) [List Operations](#) [Expand Operations](#) [Raw](#)

dataset : OpenTox Dataset service [Show/Hide](#) [List Operations](#) [Expand Operations](#) [Raw](#)

feature : OpenTox Feature service [Show/Hide](#) [List Operations](#) [Expand Operations](#) [Raw](#)

model : OpenTox Prediction Models service [Show/Hide](#) [List Operations](#) [Expand Operations](#) [Raw](#)

property : Chemical substances Properties service [Show/Hide](#) [List Operations](#) [Expand Operations](#) [Raw](#)

query : Queries [Show/Hide](#) [List Operations](#) [Expand Operations](#) [Raw](#)

compound : Chemical structures search [Show/Hide](#) [List Operations](#) [Expand Operations](#) [Raw](#)

substance : Substance search [Show/Hide](#) [List Operations](#) [Expand Operations](#) [Raw](#)

substance : Chemical Substances service [Show/Hide](#) [List Operations](#) [Expand Operations](#) [Raw](#)

- 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](#)

substanceowner : Substance owners [Show/Hide](#) [List Operations](#) [Expand Operations](#) [Raw](#)

task : OpenTox Task service (asynchronous jobs) [Show/Hide](#) [List Operations](#) [Expand Operations](#) [Raw](#)

[base url: <https://apps.ideaconsult.net/enanomapper/api-docs> , api version: 2.7.2]

Interactive API queries

substance : Chemical Substances service [Show/Hide](#) [List Operations](#) [Expand Operations](#) [Raw](#)

- 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](#)

Implementation Notes
Substance study

Response Class
Model Model Schema

```
1 {
2   "interpretation": "subject",
3   "name": "subject",
4   "parameters": "subject",
5   "protocol": "subject",
6   "reliability": "subject",
7   "role": "subject"
8 }
```

Response Content Type: application/json

Parameters

Parameter	Value	Description	Parameter Type	Data Type
uuid	NW01-02981d4-6/00-34c8-ab4b-d433a5a00865	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 URI https://apps.ideaconsult.net/enanomapper/property/UUID - see Property service	query	string
page	0	Starting page	query	int
pagesize	10	Page size	query	int

Response Messages

HTTP Status Code	Reason	Response Model
200	OK	
400	Invalid substance identifier	
404	Substance not found	
403	Forbidden	
401	Not Authorized	
405	Method not allowed	
500	Internal server error	
501	Not implemented	
503	Service unavailable	

[Try it out!](#) [Hide Response](#)

Request URL

<https://apps.ideaconsult.net/enanomapper/substance/NW01-02981d4-6/00-34c8-ab4b-d433a5a00865/study?top=P-CHEM&page=0&pagesize=10>

Response Body

```
1 {
2   "TESTPAT_FORM": null
3 },
4 {
5   "reliability": {
6     "reliability": "false",
7     "reliabilityForClassification": "false",
8     "reliabilityForQSAR": "false",
9     "purpose": null,
10    "studyResultType": "experimental result",
11    "value": null
12 },
13 },
14 {
15   "interpretation": {
16     "result": null
17 },
18 },
19 {
20   "effects": {
21     "endpoints": "PARTICLE SIZE",
22     "conditions": {
23       "result": {
24         "unit": "nm",
25         "value": 30
26       }
27 }
28 }
```

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

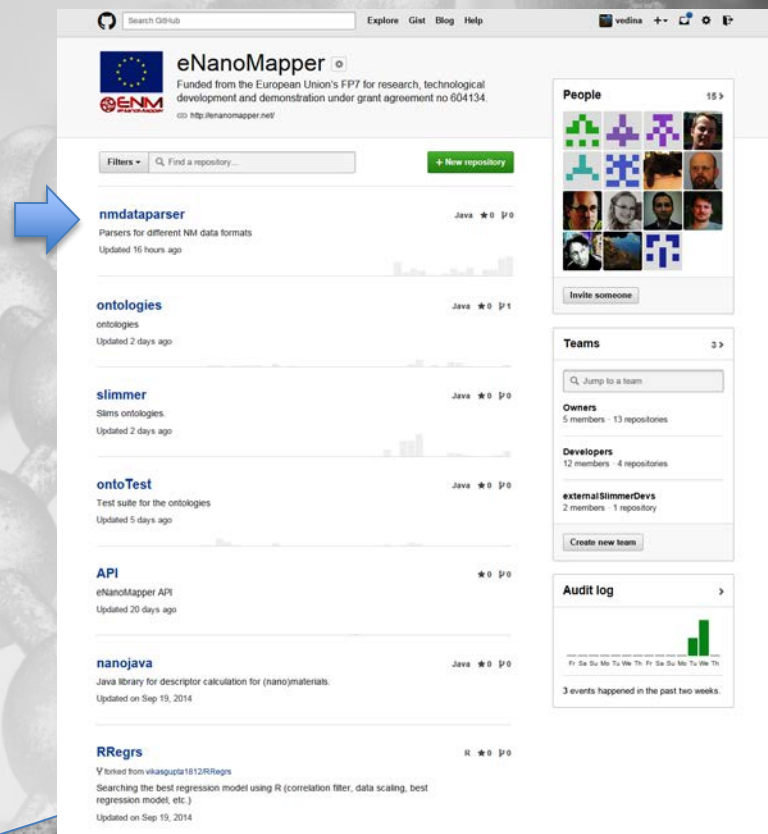


Data formats

eNanoMapper@gitHub

Import formats

- Available
 - Custom CSV
 - Custom RDF (NanoWiki)
 - IUCLID5 *.i5z
- Under development :
 - ISA-TAB-Nano parser
 - Configurable parser for spreadsheet data templates, provided by NSC projects



Data formats

enanomapper / nmdataparser

branch: master

[nmdataparser / src / test / resources / net / enanomapper / parser / csv / ProteinCoronaTest1.json](#)

214 lines (214 sloc) 7.107 kb Raw Blame History

214 lines (214 sloc) 7.107 kb Raw Blame History

214 lines (214 sloc) 7.107 kb Raw Blame History

The diagram illustrates the mapping of a JSON object to a table structure. The JSON object is shown on the left, and the corresponding tables are shown on the right. Blue arrows indicate the mapping from specific JSON objects to their respective tables.

JSON Object:

```

{
  "TEMPLATE_INFO": {
    "NAME": "ProteinCorona",
    "VERSION": "original",
    "TYPE": 1
  },
  "DATA_ACCESS": {
    "ITERATION": "ROW_SINGLE",
    "SHEET_INDEX": 1,
    "START_ROW": 13,
    "START_HEADER_ROW": 1,
    "END_HEADER_ROW": 12,
    "ALLOW_EMPTY": true,
    "RECOGNITION": "BY_INDEX"
  },
  "SUBSTANCE_RECORD": {
    "COMPANY_UUID": "A",
    "COLUMN_INDEX": "A"
  },
  "PUBLIC_NAME": {
    "COLUMN_INDEX": "A"
  },
  "OWNER_NAME": {
    "ITERATION": "ABSOLUTE_LOCATION",
    "COLUMN_INDEX": "E",
    "ROW_INDEX": 3
  }
},
"PROTOCOL_APPLICATIONS": [
  {
    "CITATION_TITLE": {
      "ITERATION": "ABSOLUTE_LOCATION",
      "COLUMN_INDEX": "E",
      "ROW_INDEX": 3
    },
    "PROTOCOL_CATEGORY_CODE": {
      "ITERATION": "ABSOLUTE_LOCATION",
      "COLUMN_INDEX": "E",
      "ROW_INDEX": 1
    },
    "PROTOCOL_GUIDELINE": {
      "guideline1": {
        "ITERATION": "ABSOLUTE_LOCATION",

```

Template Info Table:

1	A	B	C
1	EndpointCategory	Core compos	Surface modifi
2	Protocol		
3	Guideline		
4	type_of_study		
5	type_of_method		
6	data_gathering_instru	Description	
7	Endpoint	Element	Abbreviated
8	Cell		
9	MEDIUM		
10	Condition		
11	Designation		
12	Units		
13	G15.AC	[Au]	AC
14	G15.AMT	[Au]	AMT

Substance Record Table:

1	A	B	C
1	Company	Product	Product
2	Product	Product	Product
3	Product	Product	Product
4	Product	Product	Product
5	Product	Product	Product
6	Product	Product	Product
7	Product	Product	Product
8	Product	Product	Product
9	Product	Product	Product
10	Product	Product	Product
11	Product	Product	Product
12	Product	Product	Product
13	Product	Product	Product
14	Product	Product	Product
15	Product	Product	Product
16	Product	Product	Product
17	Product	Product	Product
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19	Product	Product	Product
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21	Product	Product	Product
22	Product	Product	Product
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27	Product	Product	Product
28	Product	Product	Product
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33	Product	Product	Product
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37	Product	Product	Product
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39	Product	Product	Product
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71	Product	Product	Product
72	Product	Product	Product
73	Product	Product	Product
74	Product	Product	Product
75	Product	Product	Product
76	Product	Product	Product
77	Product	Product	Product
78	Product	Product	Product
79	Product	Product	Product
80	Product	Product	Product
81	Product	Product	Product
82	Product	Product	Product
83	Product	Product	Product

Parser for (mainly)
spreadsheet data templates
(under development)

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	EndpointCategory	Core compos	Surface modifie	External Iden	Cell.association					PC GRANULOMETRY	PC GRANULOMETRY					PC GRANU
2	Protocol				ICP-AES					TEM	TEM					DLS
3	Guideline				doi:10.1021/r											doi:10.102
4	type_of_study				ICP-AES											
5	type_of_method				Perkin-Elmer					TEM	TEM					DLS
6	data_gathering_instru	Description								Tecnaai 20	Tecnaai 20	Tecnaai 20 (FEI)	microscope	AMT 16000	car ZetaSizer	2
7	Endpoint	Element	Abbreviated	Classification	Net cell assoc	Net cell a	Net cell a	Log2 trans	Log2 trans	Core size		Density	MW	Mol/NP	SA/NP	Z-Average
8	Cell				AS49	AS49	AS49	AS49	AS49							
9	MEDIUM															
10	Condition															
11	Designation				Mean	SD	N	Mean	SD	Mean	SD				Mean	
12	Units				mL/(ug(Mg)	1/ug(Mg)				nm	nm	g/cm^3	g/mol		cm^2/NP	nm
13	G15.AC	[Au]	AC	Anionic	0.02751	0.01654	3	-5.184	0.867	14.9	1.2	19.1	197	0	0	22.36
14	G15.AHT	[Au]	AHT	Cationic	0.49705	0.08013	3	-1.009	0.233	14.9	1.2	19.1	197	0	0	30.59

[illegible]

Page	Page No.	Page Title	Page Content
1	1	1	1
2	2	2	2
3	3	3	3
4	4	4	4
5	5	5	5
6	6	6	6
7	7	7	7
8	8	8	8
9	9	9	9
10	10	10	10
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77	77	77	77
78	78	78	78
79	79	79	79
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81	81	81	81
82	82	82	82
83	83	83	83
84	84	84	84
85	85	85	85
86	86	86	86
87	87	87	87
88	88	88	88
89	89	89	89
90	90	90	90
91	91	91	91
92	92	92	92
93	93	93	93
94	94	94	94
95	95	95	95
96	96	96	96
97	97	97	97
98	98	98	98
99	99	99	99
100	100	100	100

Questions?

THANK YOU!