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

NINA JELIAZKOVA
IdeaConsult Ltd.
Sofia, Bulgaria
www.ideaconsult.net

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

Karolinska Institutet

Maastricht University Leading in Learning!

EMBL-EBI

Douglas Connect GmbH

in silico toxicology gmbh

IDEA consult

Nat. Tech. Univ. of Athens, Greece

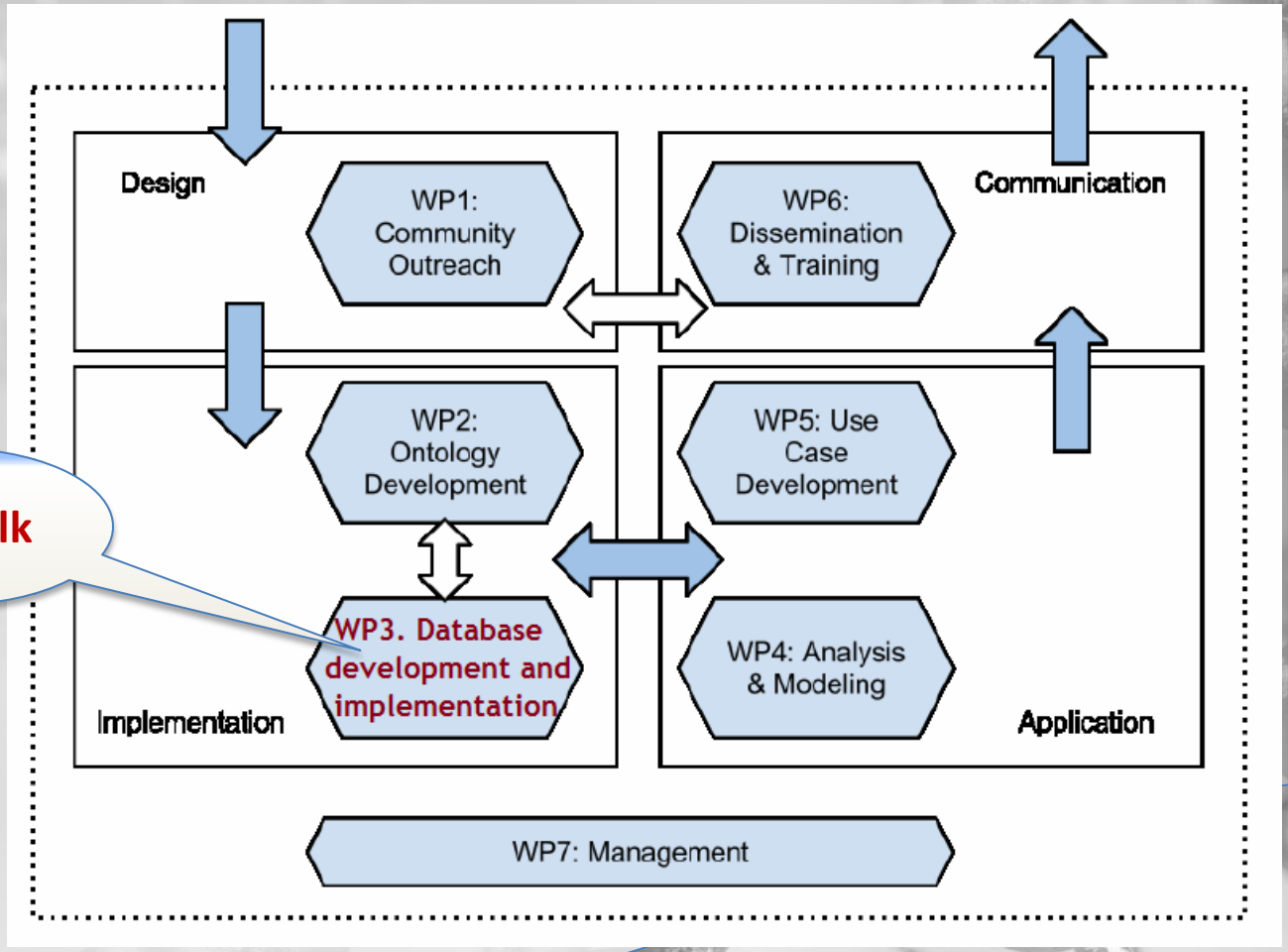
eNanoMapper

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, …)

eNanoMapper

Work packages



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

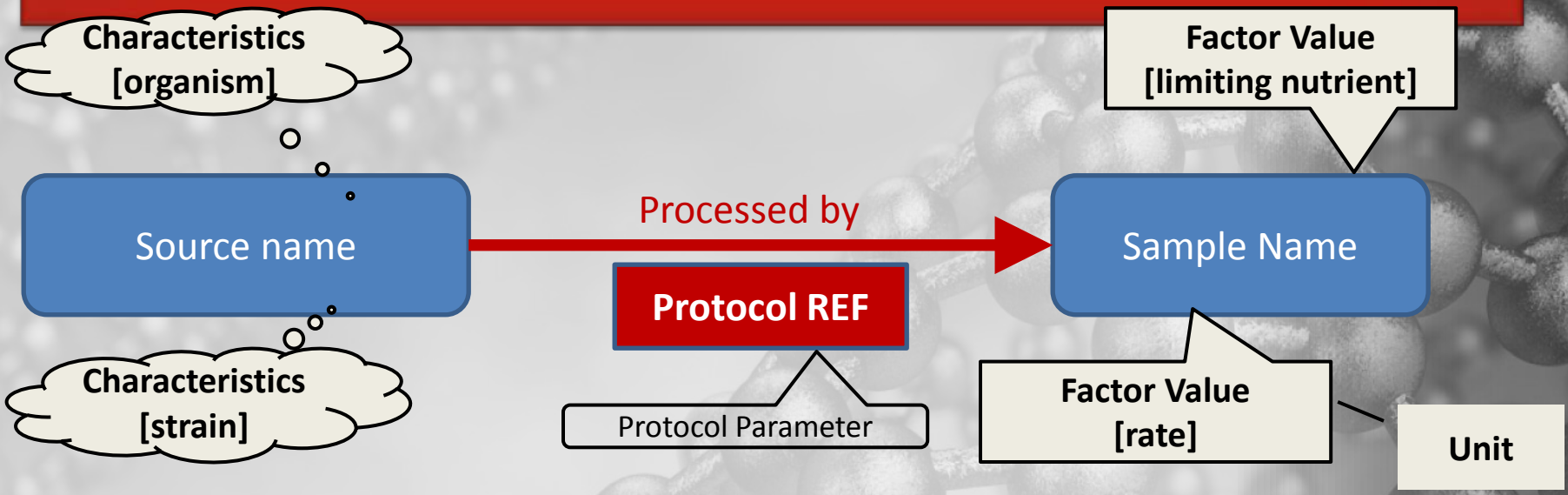
- Database dumps : 3
- ISA-Tab-Nano format : 1
- IUCLID5 format : 1
- Semantic MediaWiki : 1
- Programmatic access through a publicly available API : 4
- Only one source makes distinction between raw and processed data and provides access to both types of data.

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

The Experimental graph



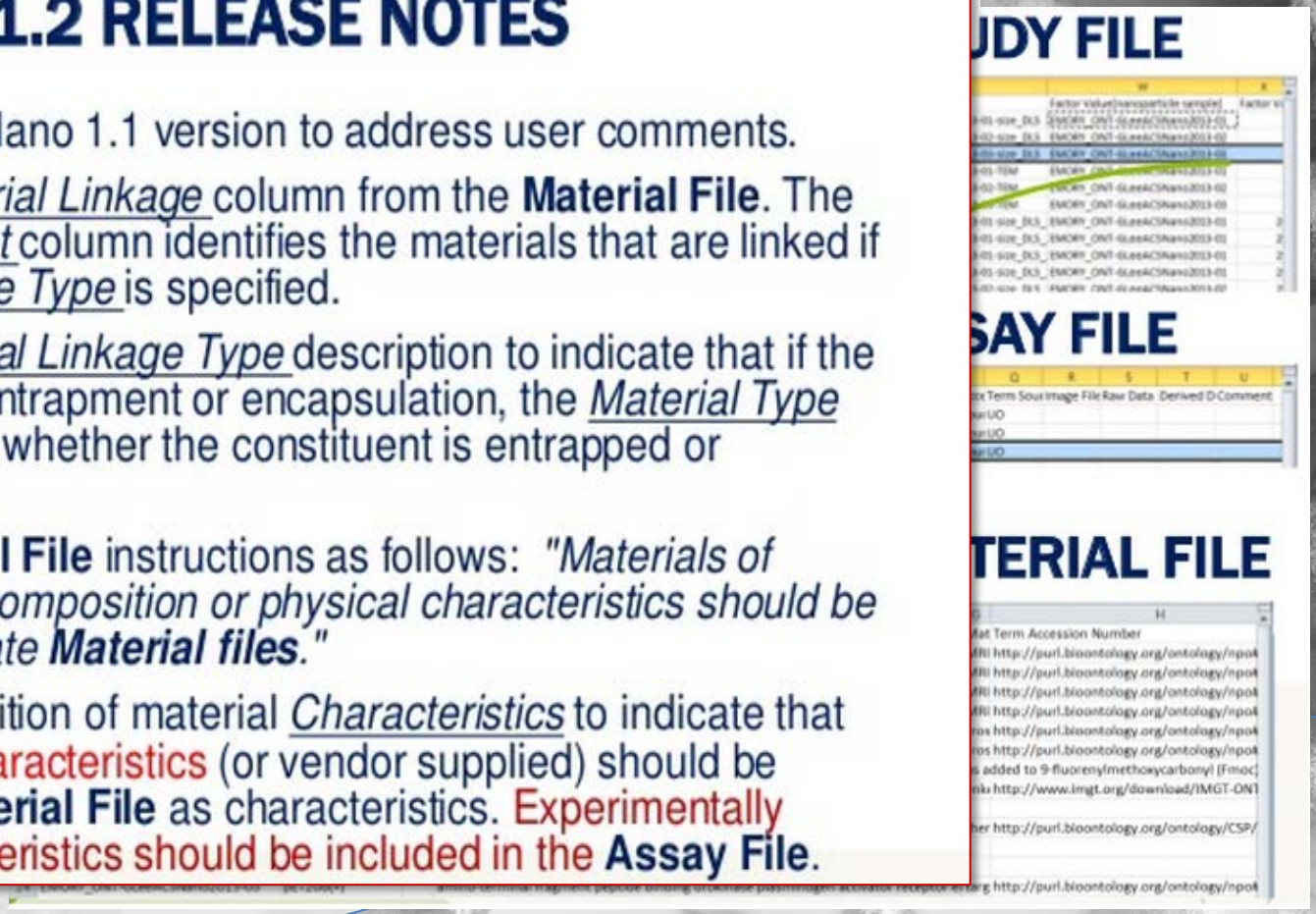
Source Name	Characteristics [organism]	Characteristics [strain]	Protocol REF	Sample Name	Factor Value [limiting nutrient]	Factor Value [rate]	Unit
culture1	Saccharomyces cerevisiae	FY1679	growth protocol	C-0.07-aliquot1	carbon	0.07	l/hour
culture4	Saccharomyces cerevisiae	FY1679	growth protocol	N-0.07-aliquot1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

ISA-TAB-Nano

ISA-TAB-NANO 1.2 RELEASE NOTES

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

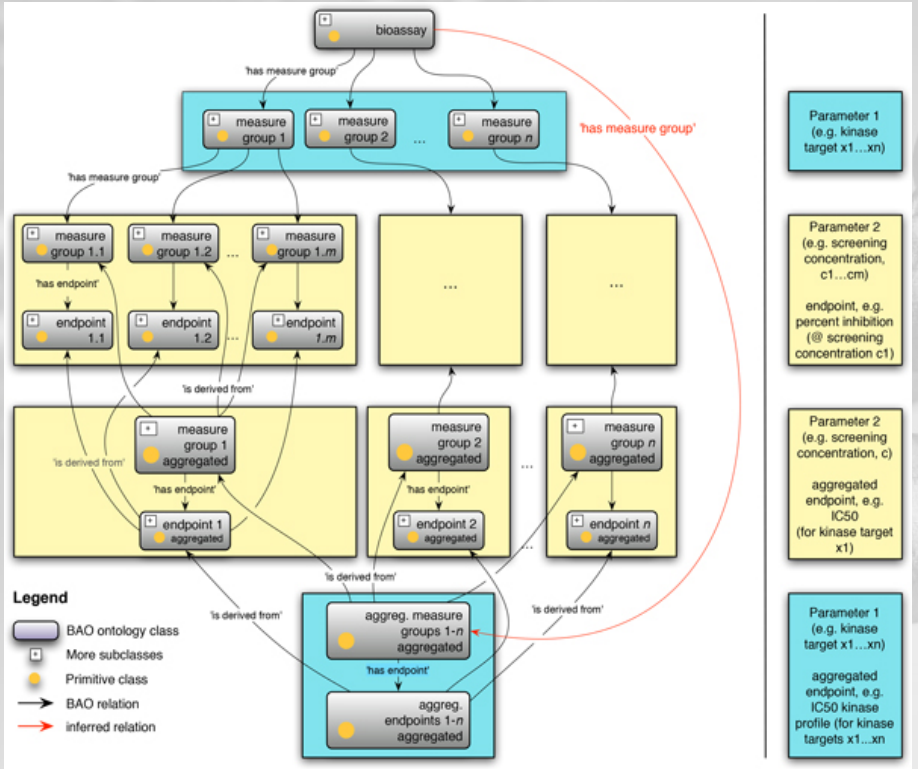
- Removed the *Material Linkage* column from the **Material File**. The *Material Constituent* column identifies the materials that are linked if the *Material Linkage Type* is specified.
- Modified the *Material Linkage Type* description to indicate that if the linkage type is an entrapment or encapsulation, 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**.



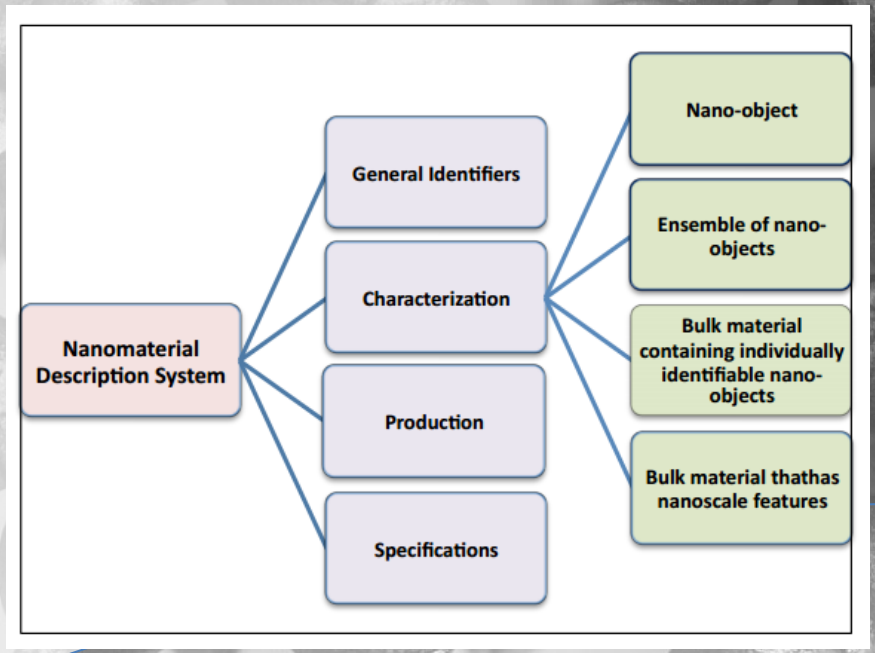
eNanoMapper

Existing data models (cont)

BioAssay Ontology



CODATA Uniform Description System for Materials at the Nanoscale



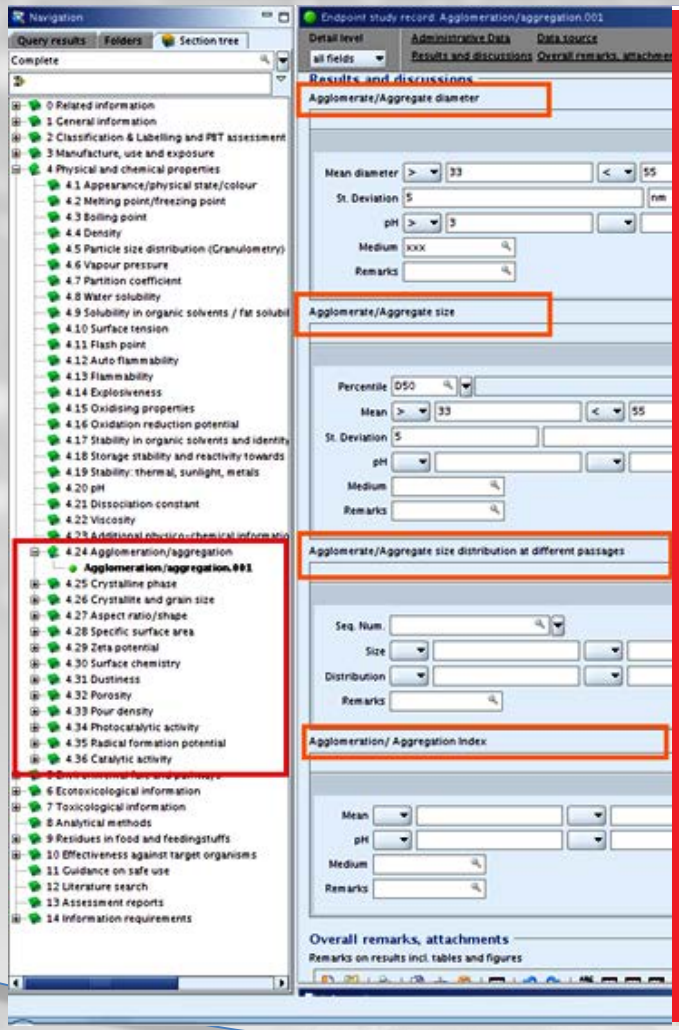
eNanoMapper

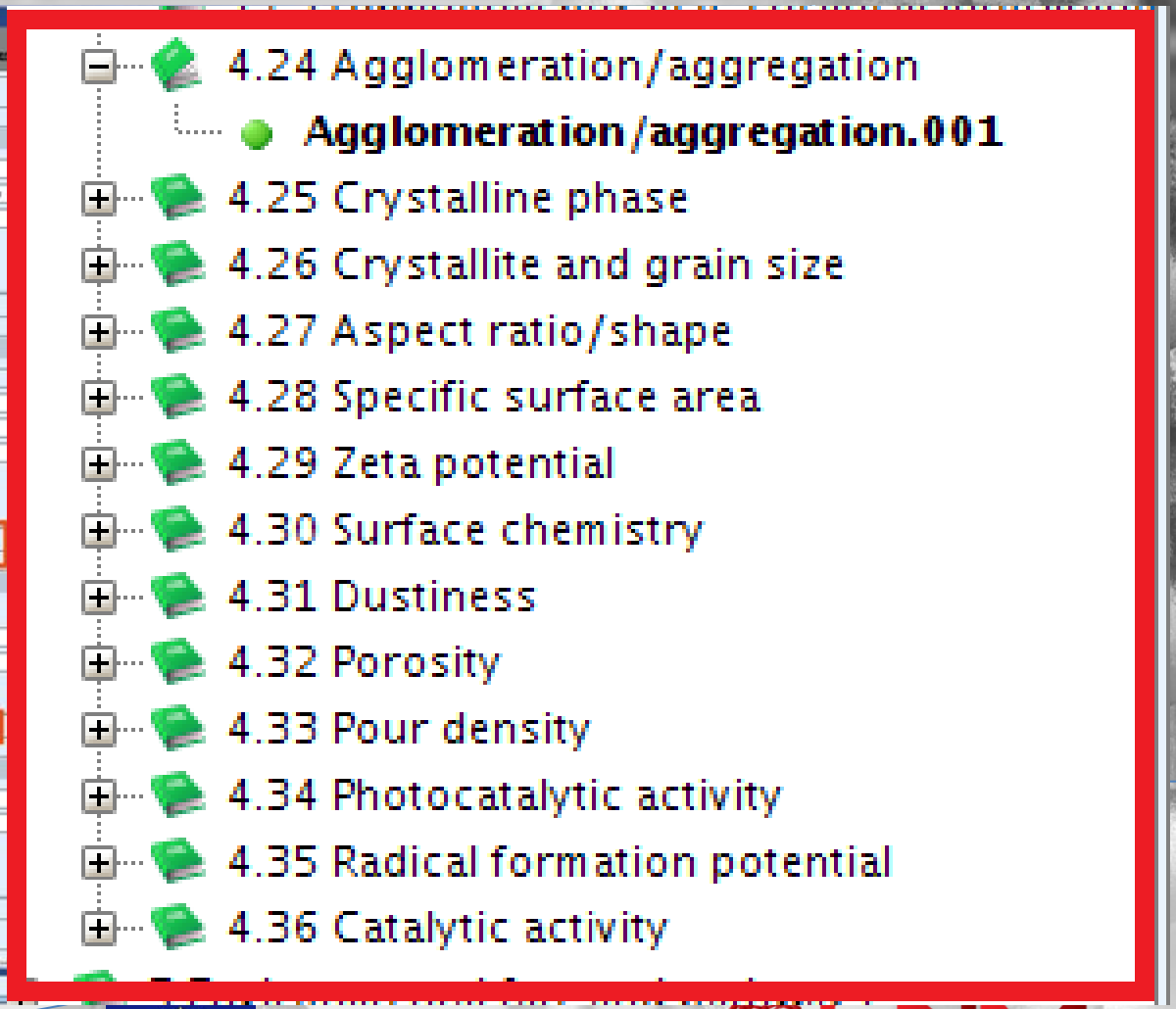
Experimental data

- **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





eNanoMapper

Chemical /Toxicogenomics DB
(no explicit NM support)

PubChem 10 Years

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

ChEMBL

NM: Fullerenes , Metal oxides

ArrayExpress

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

ctd™

Comparative Toxicogenomics Database
Includes nanomaterial related data.

ECHA EUROPEAN CHEMICALS AGENCY

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

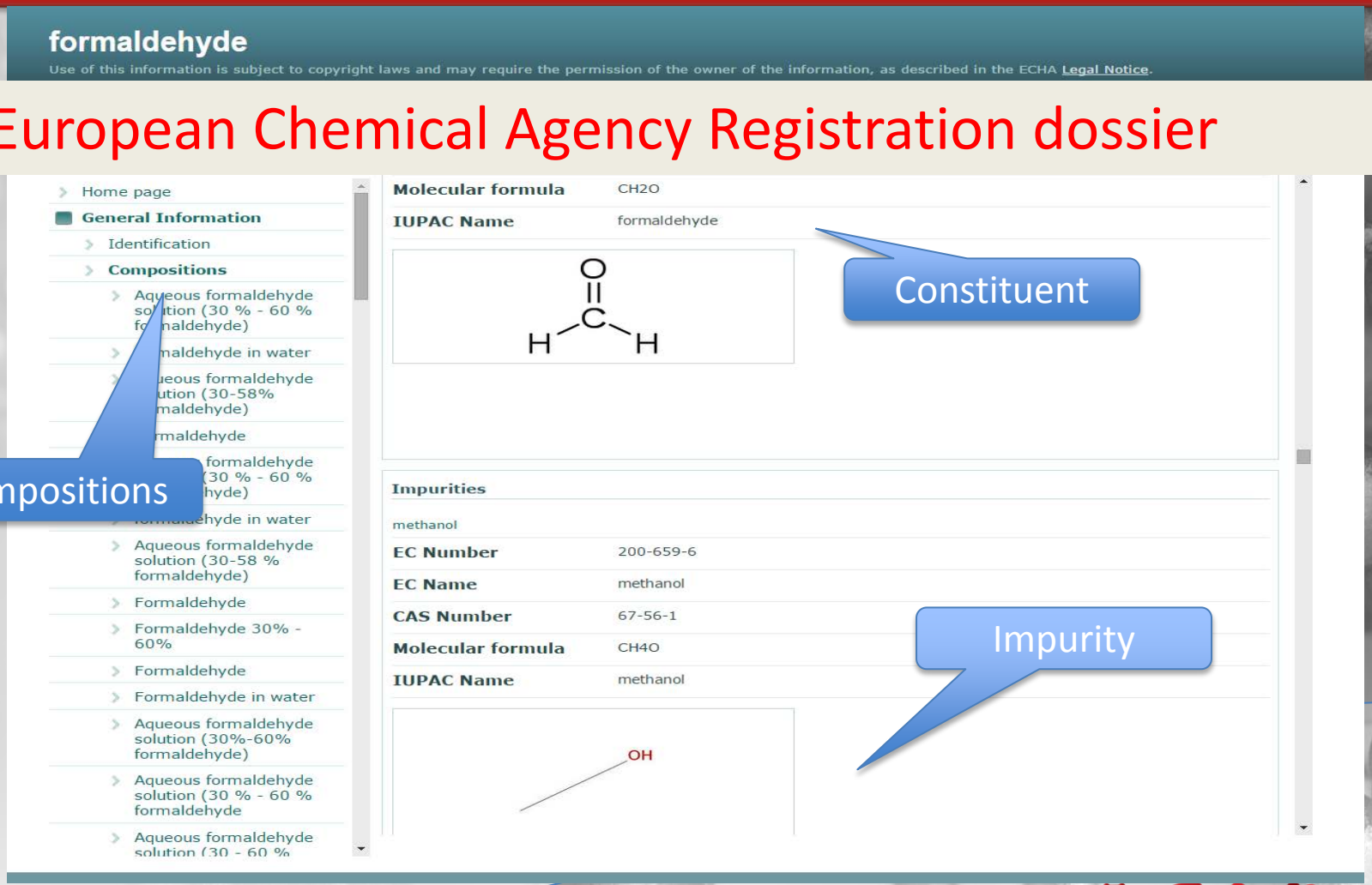
- Chemical structure and properties

- 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)



Substance (25155-25-3)

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

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

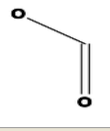
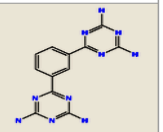
Reaction mass of ....

Multi constituent substance

Substance (formaldehyde)

	Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info
- 1 -	formaldehyde (IUC4 DSN 52)	IUC4-efdb21bb-e7...	Existing Chemical		ECB5-053aa8c4-d...	OECD / Paris / France	IUCLID4 = DSN 52

Composition name: Other: Sales Products In Aqueous Solution
Composition UUID: L-cf10d721-b0e7-37cd-a233-e9a2483c4d3c
Purity of IUC Substance:

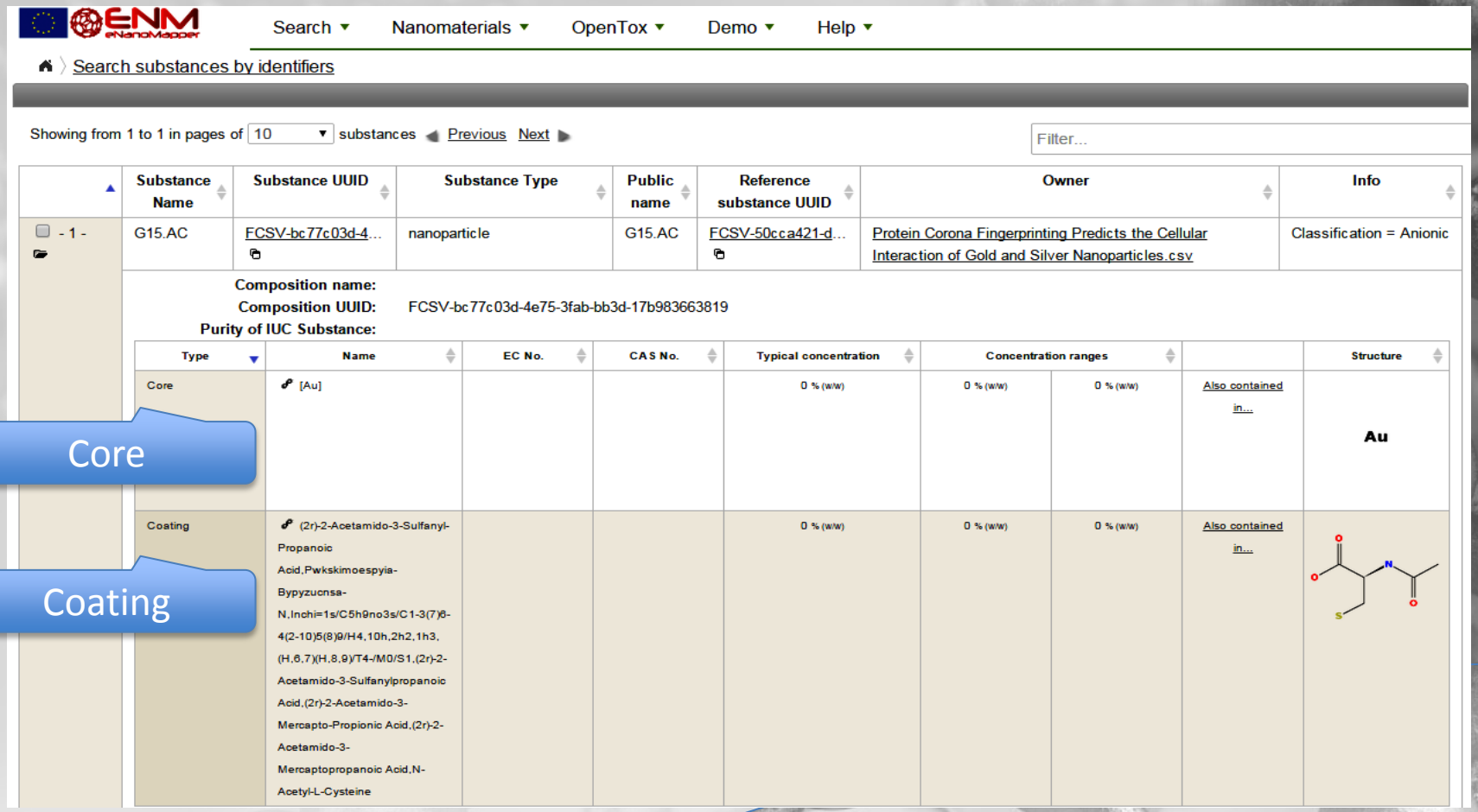
Type	Name	EC No.	CAS No.	Typical concentration	Concentration ranges			Structure
Constituent	Formaldehyde	200-001-8	50-00-0	0 % (w/w)	0 % (w/w)	0 % (w/w)	Also contained in...	
Impurity	Formic Acid	200-579-1	64-18-6	ca.0.3 % (w/w)	0 % (w/w)	0 % (w/w)	Also contained in...	
Impurity	Iron,Iron(2+)	231-096-4	7439-89-6	<=0.0001 % (w/w)	0 % (w/w)	0 % (w/w)	Also contained in...	
Impurity	Methanol	200-659-6	67-56-1	0 % (w/w)	0.5 % (w/w)	2 % (w/w)	Also contained in...	
Additive	6-[3-[4,6-Bis(Azanyl)-1,3,5-Triazin-2-Yl]Phenyl]-1,3,5-Triazine-2,4-Diamine,Svofltdqizskln-Uhfffaoysa-N,Inchi=1s/C12h12n10/C13-9-	225-859-0	5118-80-9	0 % (w/w)	0 % (w/w)	0 % (w/w)	Also contained in...	
Additive (solvent)	Water	231-791-2	7732-18-5	ca.49 % (w/w)	0 % (w/w)	0 % (w/w)	Also contained in...	

Constituent

Impurity

Additive

Gold nanoparticle



eNanoMapper

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
- 1 -	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

Composition name:
Composition UUID: FCSV-bc77c03d-4e75-3fab-bb3d-17b983663819
Purity of IUC Substance:

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...	Au
Coating	(2r)-2-Acetamido-3-Sulfanyl-Propanoic Acid,Pwkskimoespyia-Bypyzucnsa-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,(2r)-2-Acetamido-3-Sulfanylpropanoic Acid,(2r)-2-Acetamido-3-Mercapto-Propionic Acid,(2r)-2-Acetamido-3-Mercaptopropanoic Acid,N-Acetyl-L-Cysteine			0 % (w/w)	0 % (w/w)	0 % (w/w)	Also contained in...	

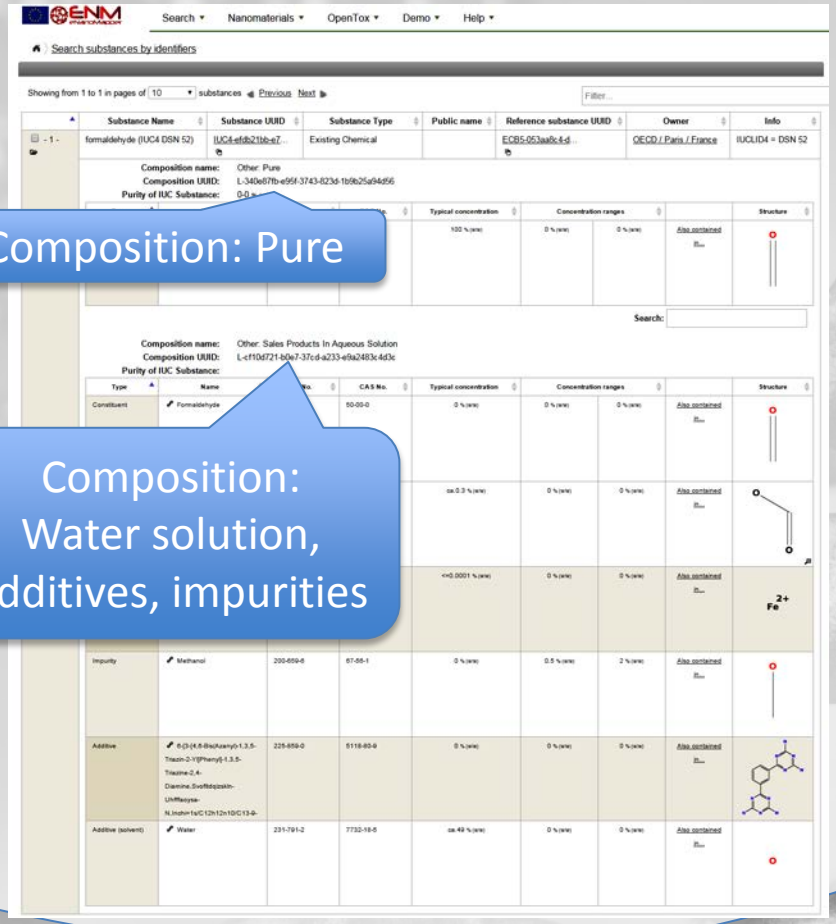
Core

Coating

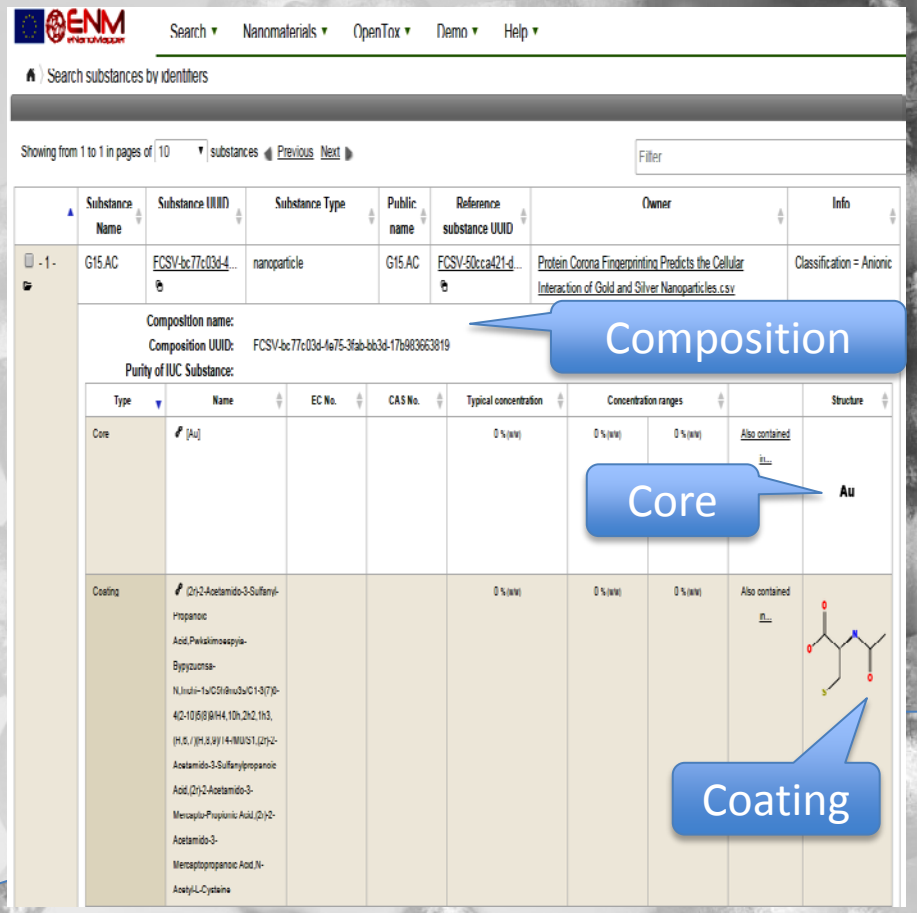
eNanoMapper

Substance, Material, Composition

Substance (formaldehyde)



Gold Nanoparticle



What we need to describe NM and related experiments

Unique identifier

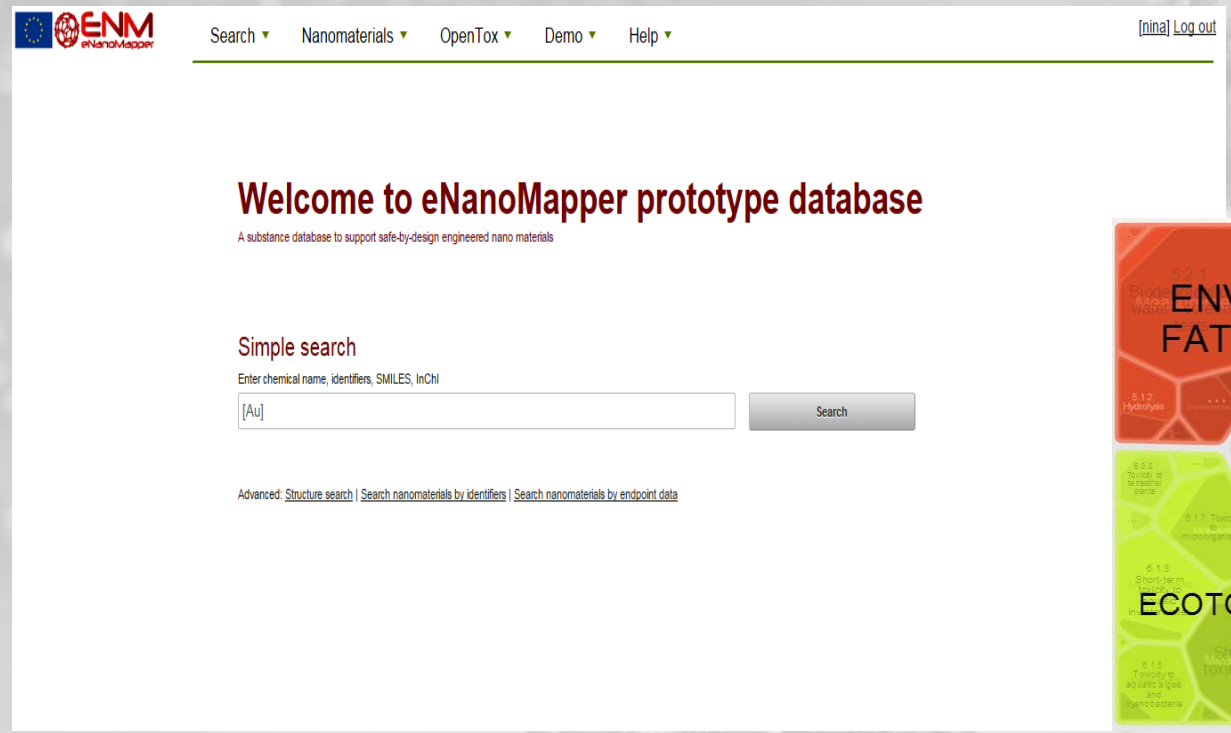
Substance / Material (composition, linkage)

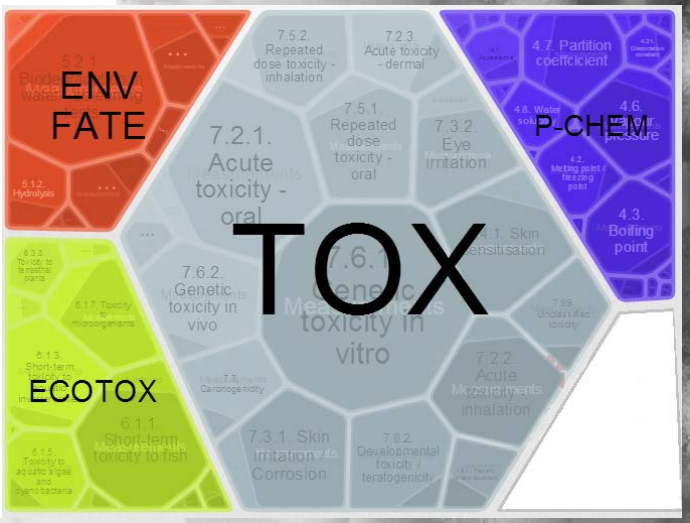
Measurements (Protocol, parameters, raw data, derived data)

What we need to describe a nanomaterial and related experiments

- **A.** An ... of the manufacturer ... 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 FUTURENANONEEDS project.
- **B.** ...
- **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 ...
- **B.2** ... where relevant (e.g. silver nano particle - linked to Ag - as in OpenTox Compounds 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 ... (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.** ...
- **C.2.** Experiment ...
- **C.3.** Experiment readouts/results
- **C.4.** Reliability
- **D.** ...

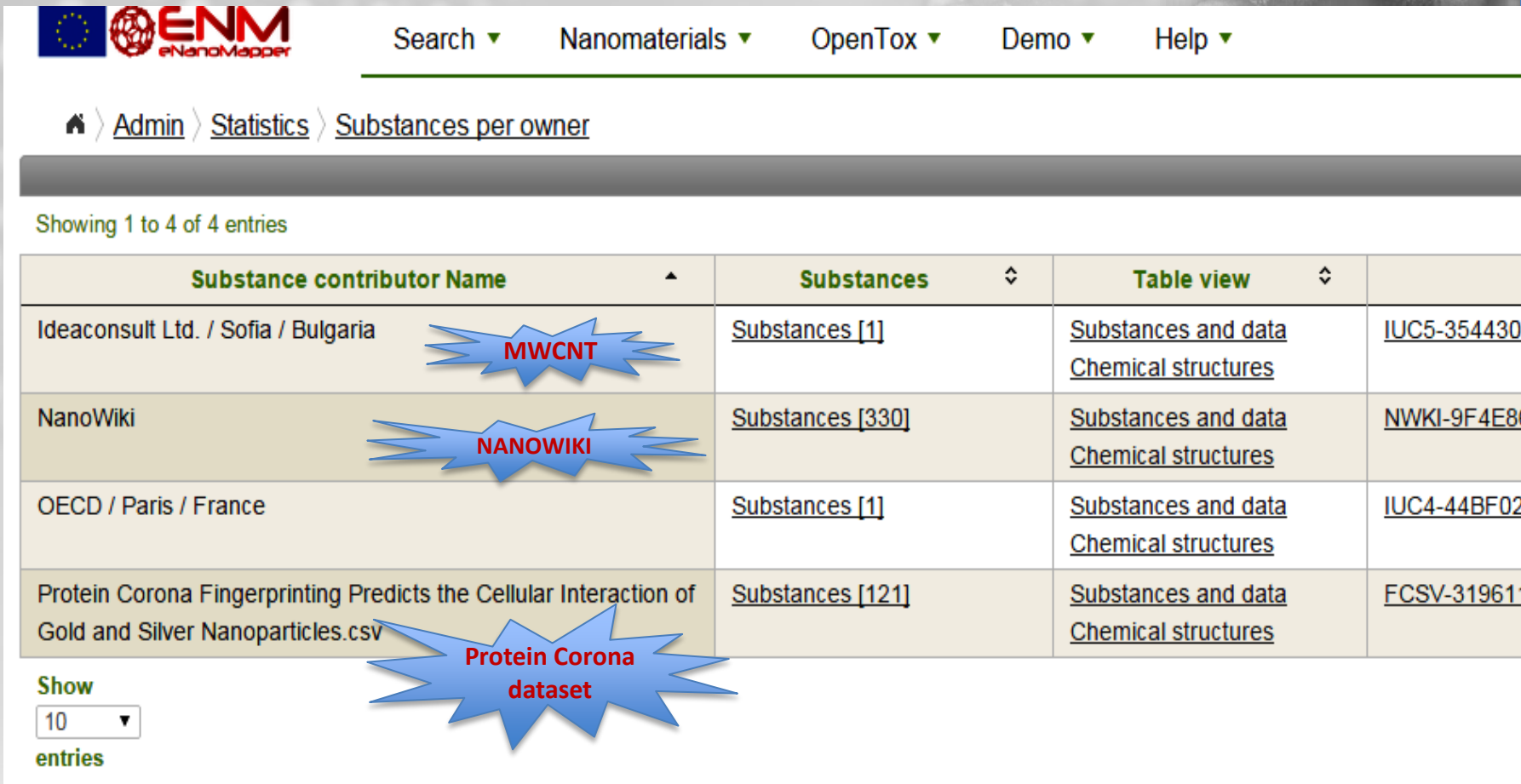
eNanoMapper prototype database



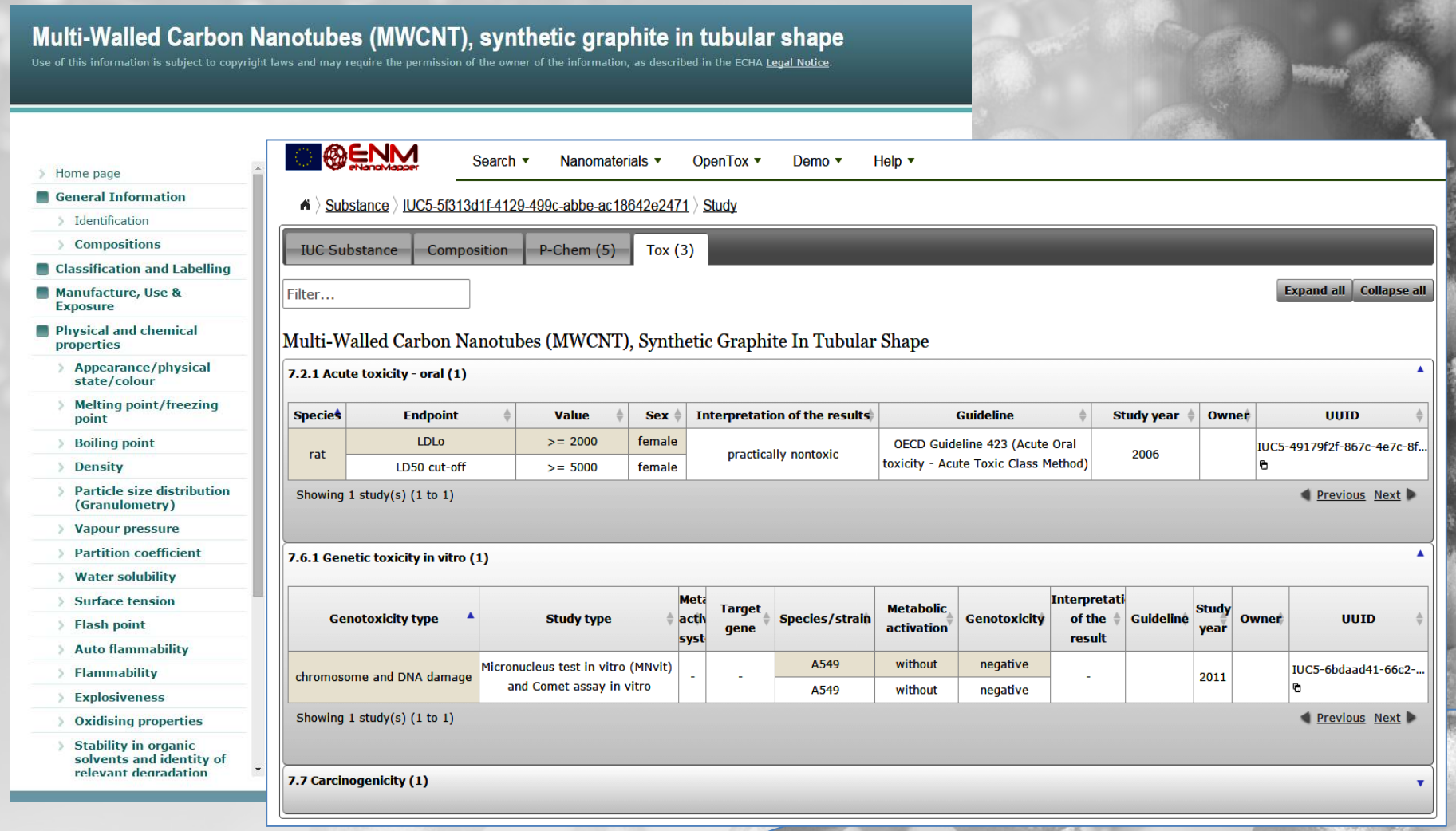


REST API documentation:
http://enanomapper.github.io/API/

Nanomaterials overview



Multi-Walled Carbon Nanotubes



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

- 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 ▶

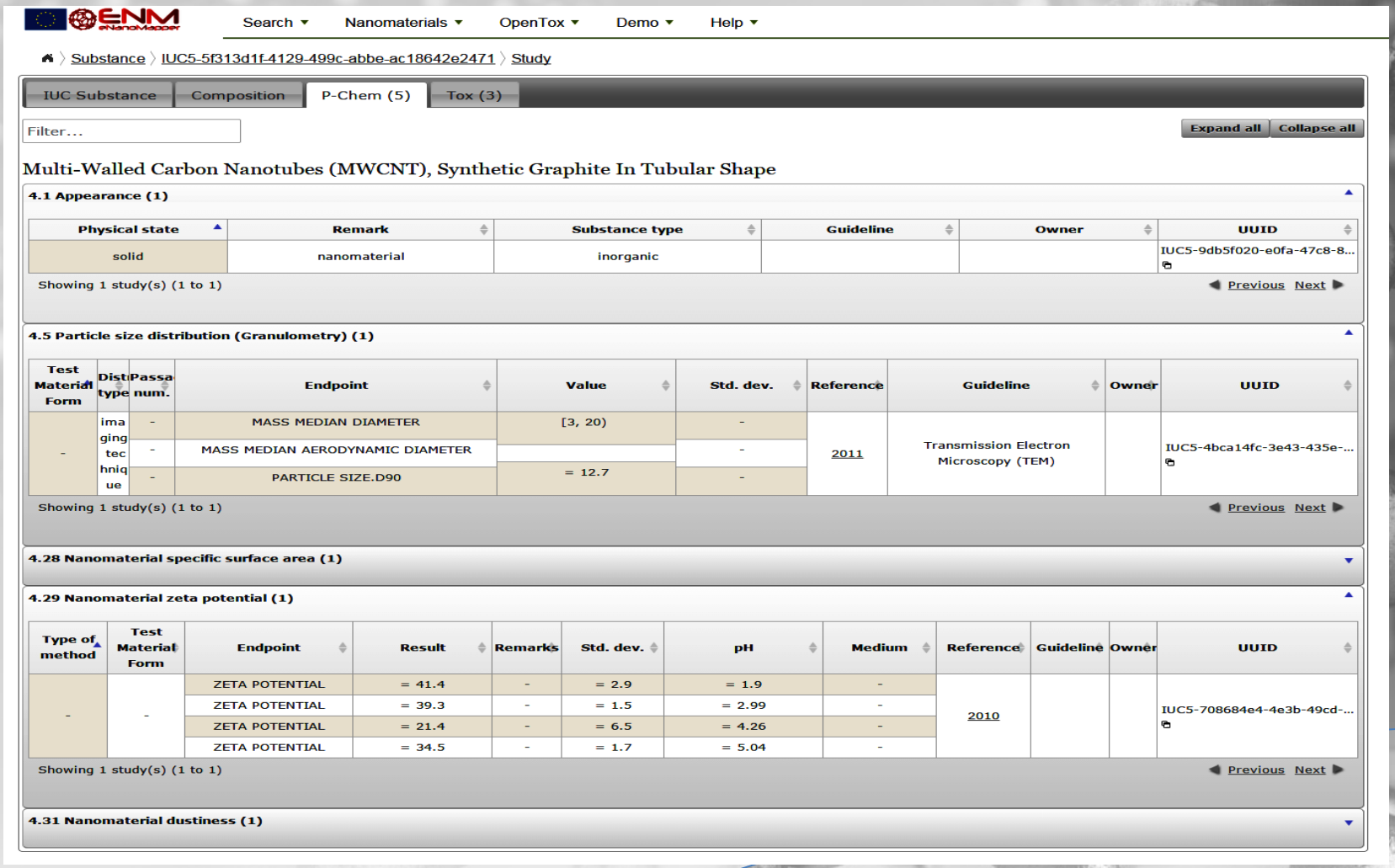
7.6.1 Genetic toxicity in vitro (1)

Genotoxicity type	Study type	Meta activ syst	Target gene	Species/strain	Metabolic activation	Genotoxicity	Interpretati 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)



eNM eNanoMapper | 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

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	Passa num.	Endpoint	Value	Std. dev.	Reference	Guideline	Owner	UUID
-	imaging technique	-	MASS MEDIAN DIAMETER	[3, 20)	-	2011	Transmission Electron Microscopy (TEM)		IUC5-4bca14fc-3e43-435e-...
		-	MASS MEDIAN AERODYNAMIC DIAMETER		-				
		-	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)

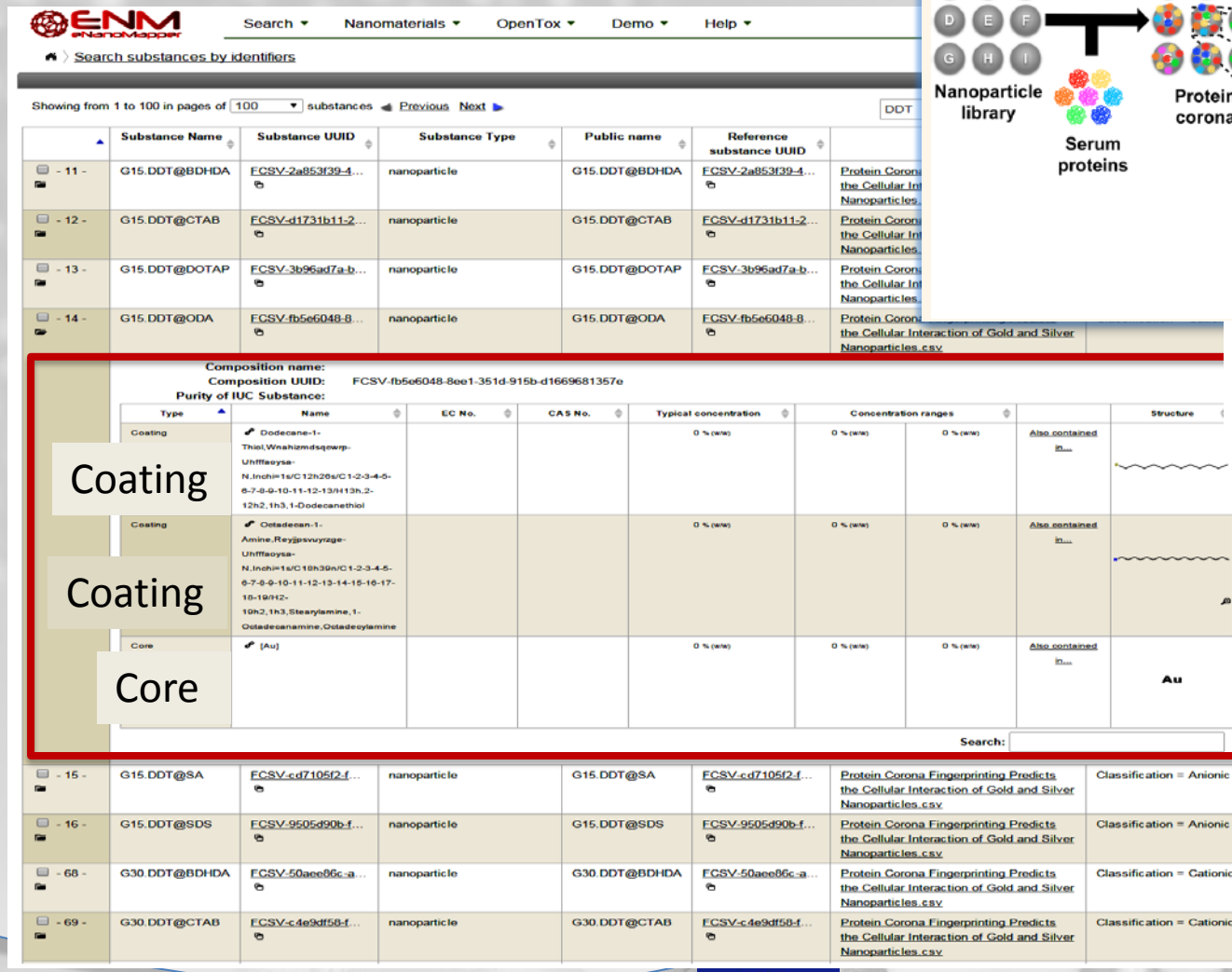
Type of method	Test Material Form	Endpoint	Result	Remarks	Std. dev.	pH	Medium	Reference	Guideline	Owner	UUID
-	-	ZETA POTENTIAL	= 41.4	-	= 2.9	= 1.9	-	2010			IUC5-708684e4-4e3b-49cd-...
		ZETA POTENTIAL	= 39.3	-	= 1.5	= 2.99	-				
		ZETA POTENTIAL	= 21.4	-	= 6.5	= 4.26	-				
		ZETA POTENTIAL	= 34.5	-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

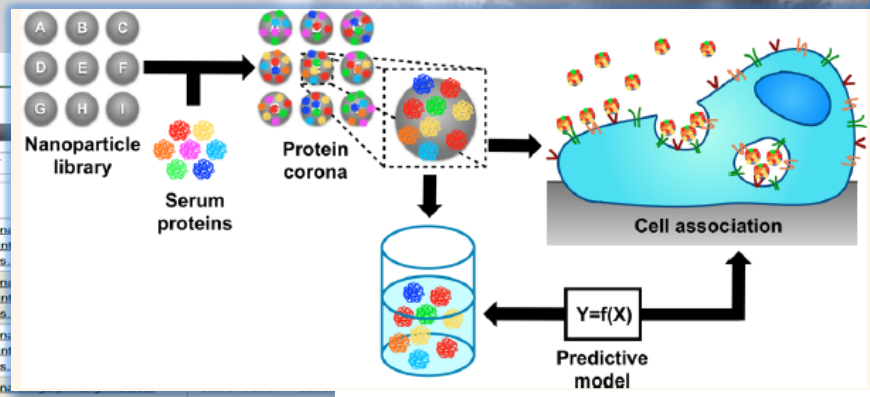
Showing 1 study(s) (1 to 1) ◀ Previous Next ▶

4.31 Nanomaterial dustiness (1)

eNM eNanoMapper

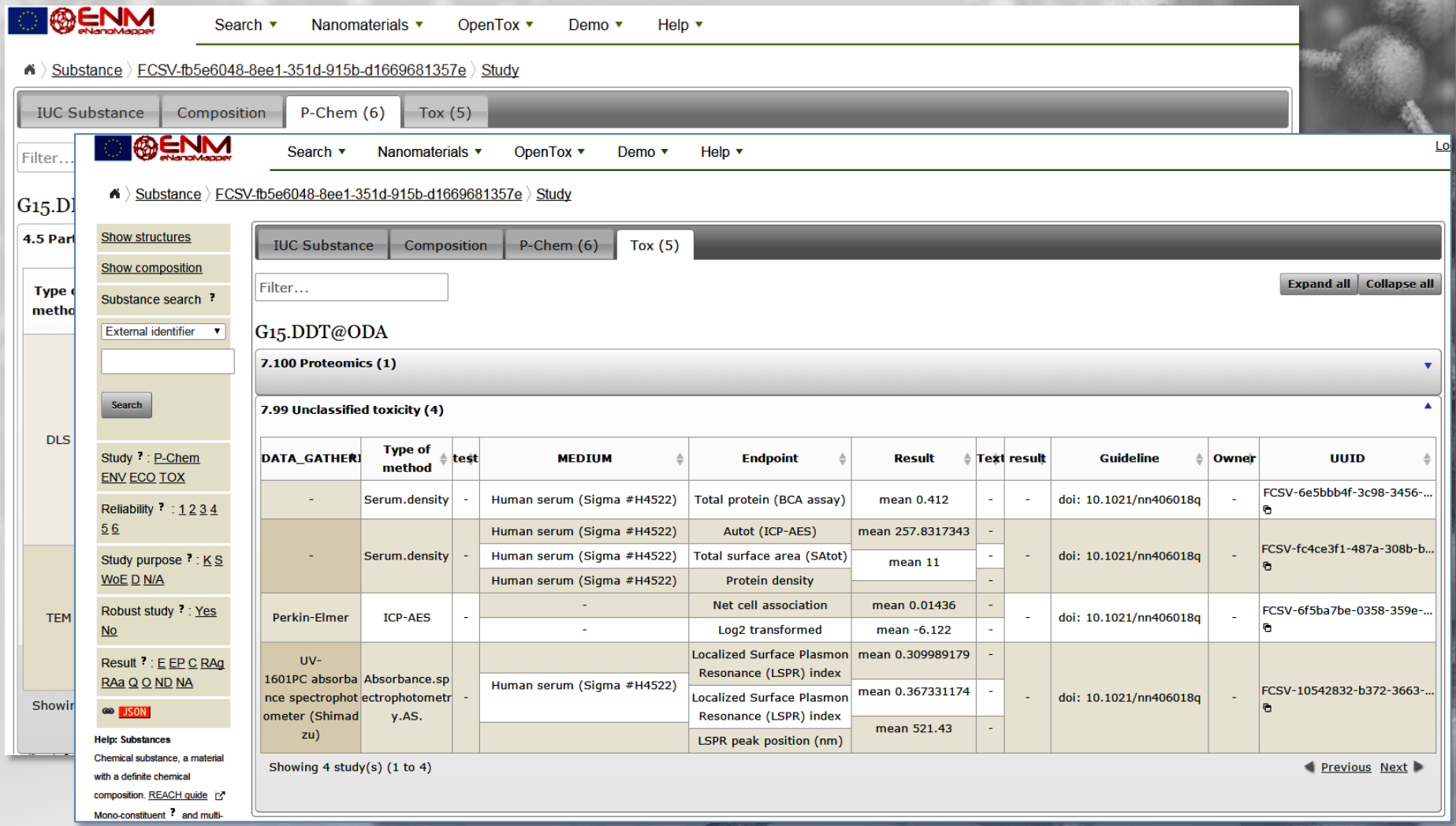
Prototype database (Protein Corona)



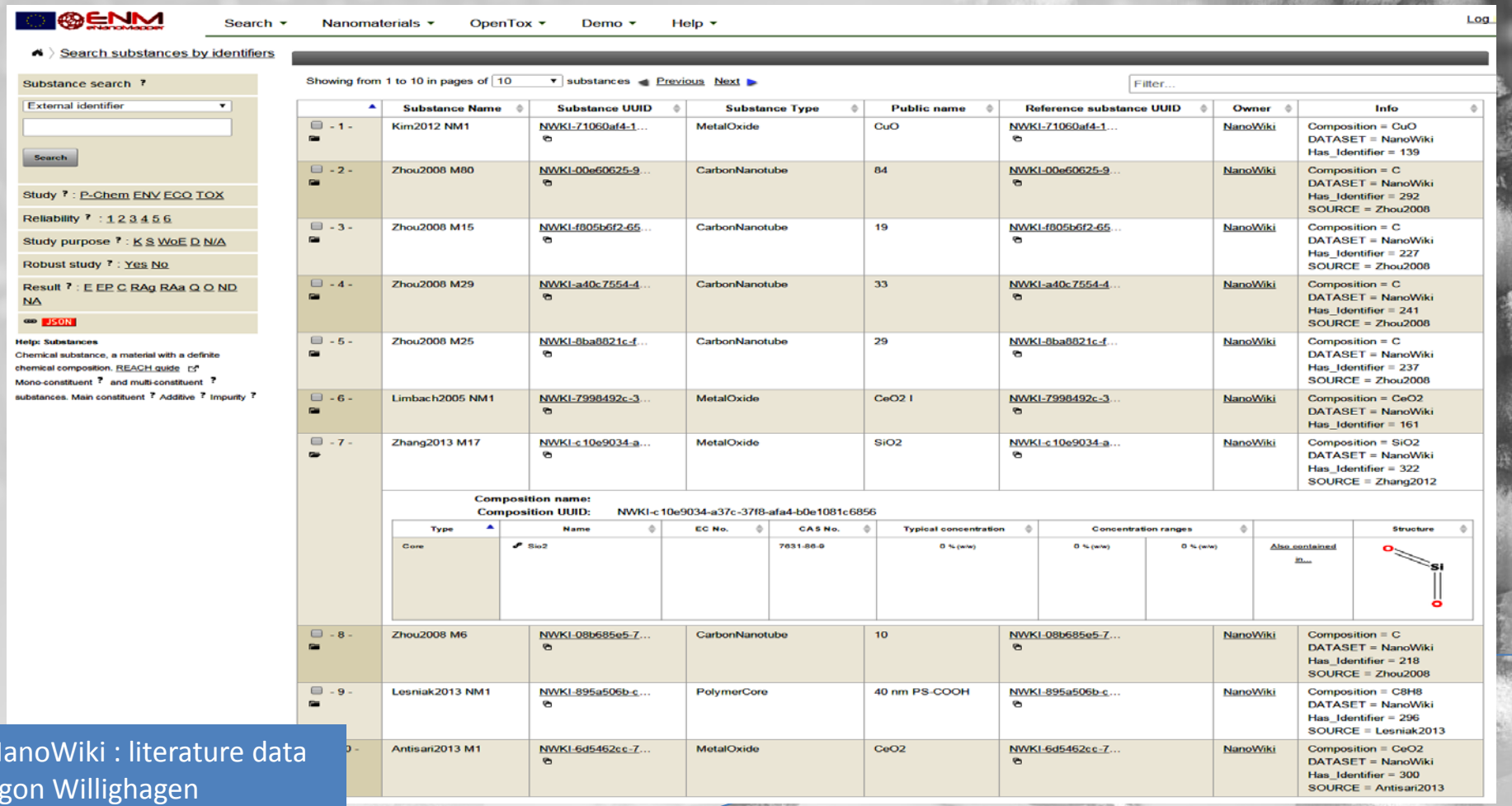


Protein Corona Data set
DOI:10.1021/nn406018q

Prototype database (Protein Corona)



Prototype database (NanoWiki)



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

NM components (NanoWiki)

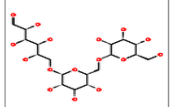
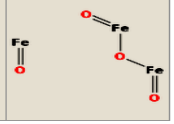
Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

Search substances by identifiers

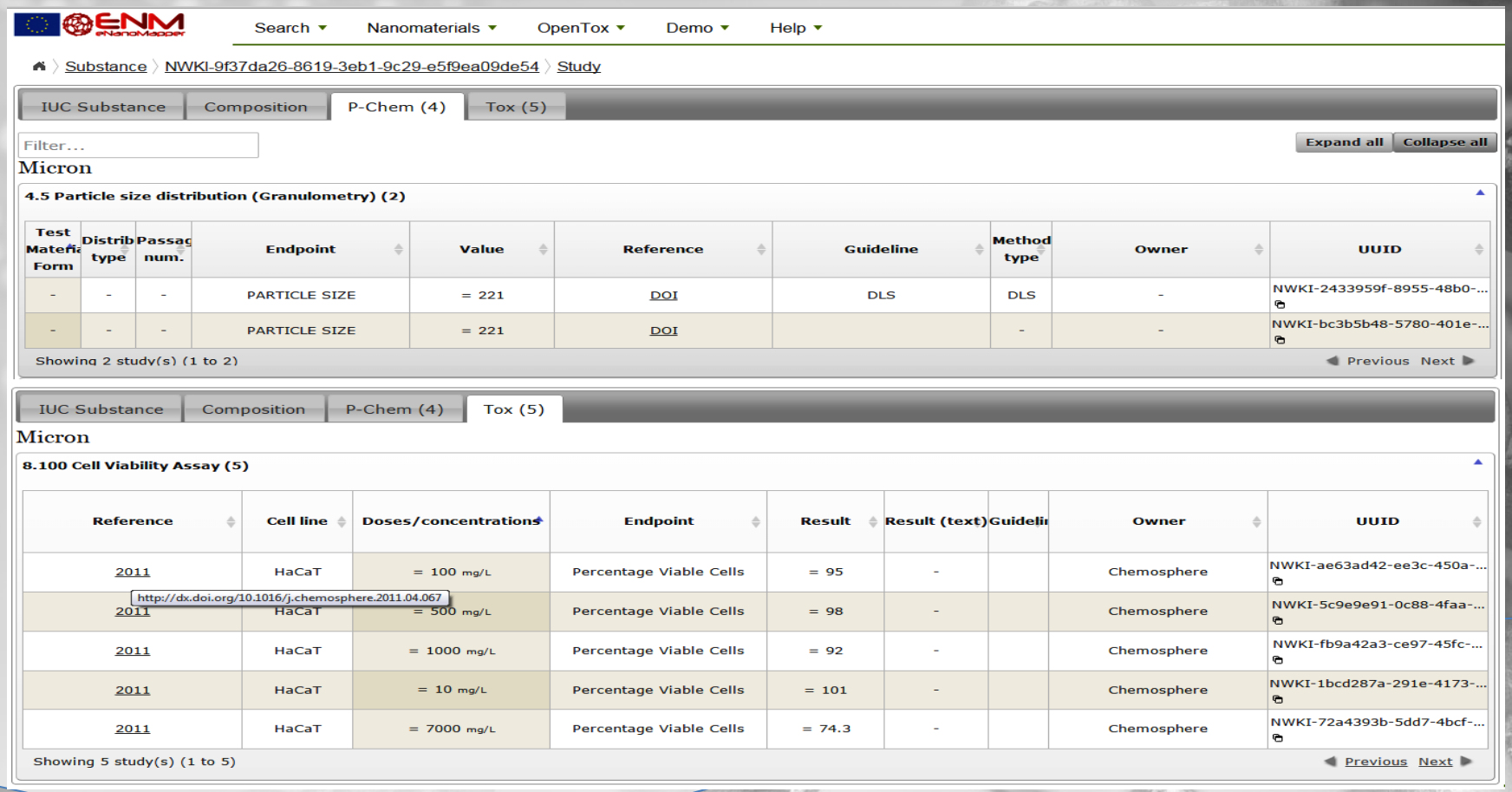
	Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info
- 1 -	Shaw51 45	NWKI-02981dd4-b...	MetalOxide	MION-47 no. 35	NWKI-02981dd4-b...	NanoWiki	Alternative Identifier = NP45 Coating = DextranCoating Composition = Fe3O4 DATASET = NanoWiki Has_Identifier = 75

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-Yl]Oxymethyl]-3,4,5-Tris(Oxidanyl)Oxan-2-Yl]Oxy-2,3,4,5-Tetrakis(Oxidanyl)Hexanal,Fzwbnhmxjmcxlu-Blaupyhcsa-N,Inchi=1s/C18h32o16/C19-1-5(21)9(23)10(24)8(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-Yl]Oxymethyl]Tetrahydropyran-2-Yl]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-Yl]Oxymethyl]Oxan-2-Yl]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-Yl]Oxymethyl]Tetrahydropyran-2-Yl]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)



eNM eNanoMapper

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 Materia 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

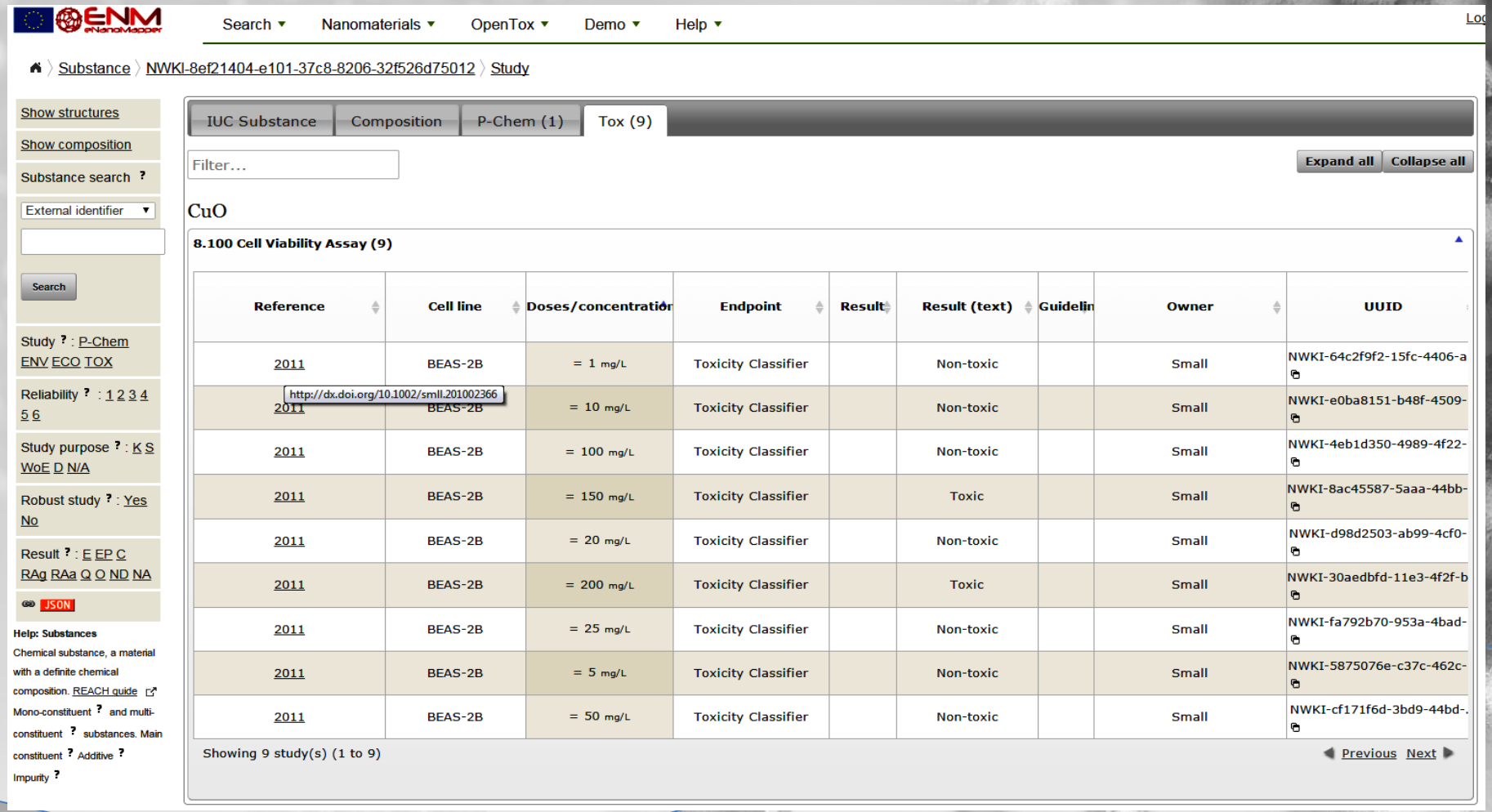
8.100 Cell Viability Assay (5)

Reference	Cell line	Doses/concentrations	Endpoint	Result	Result (text)	Guideli	Owner	UUID
2011	HaCaT	= 100 mg/L	Percentage Viable Cells	= 95	-		Chemosphere	NWKI-ae63ad42-ee3c-450a-...
2011	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-...

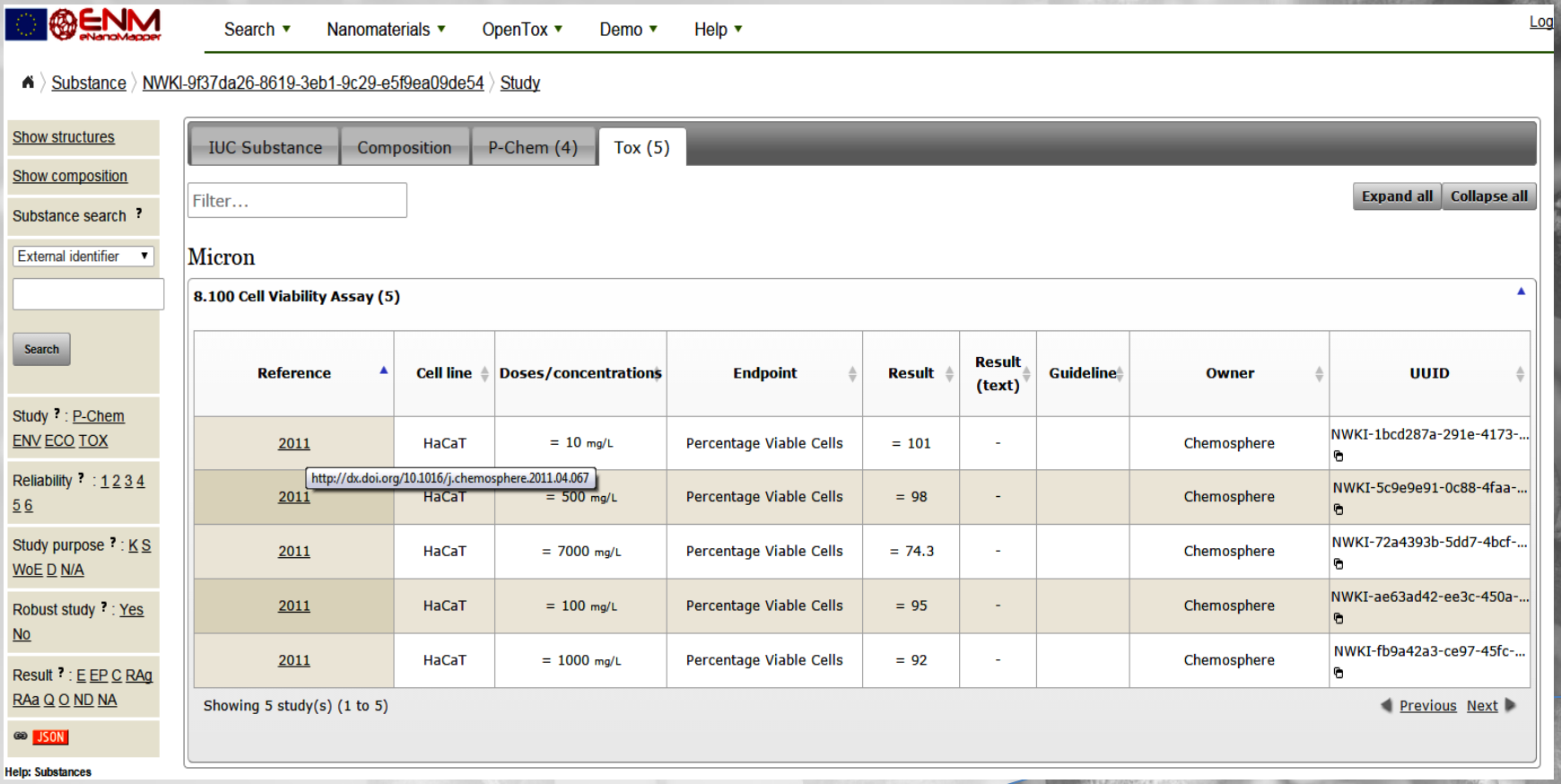
http://dx.doi.org/10.1016/j.chemosphere.2011.04.067

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

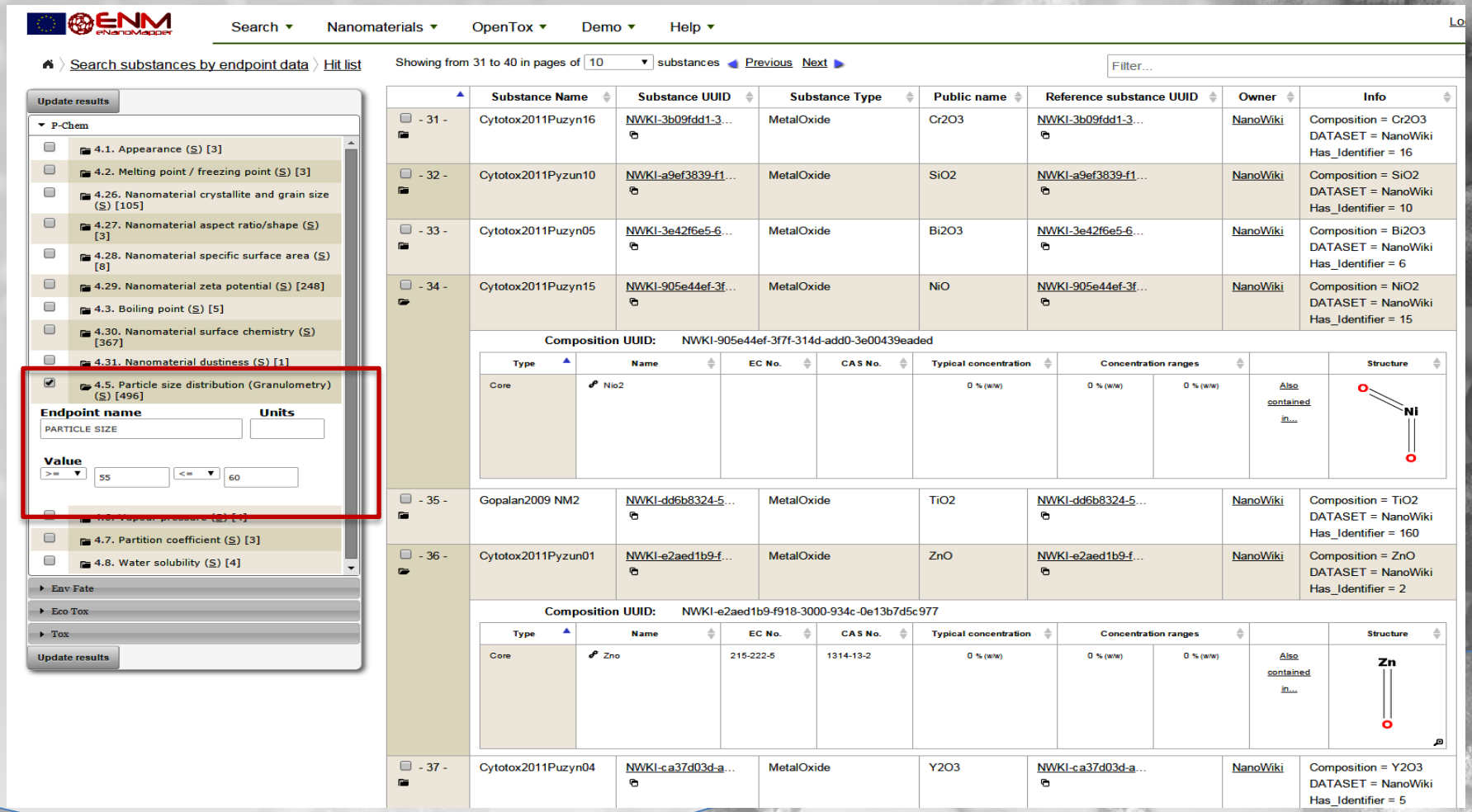
NM toxicity (classifier)



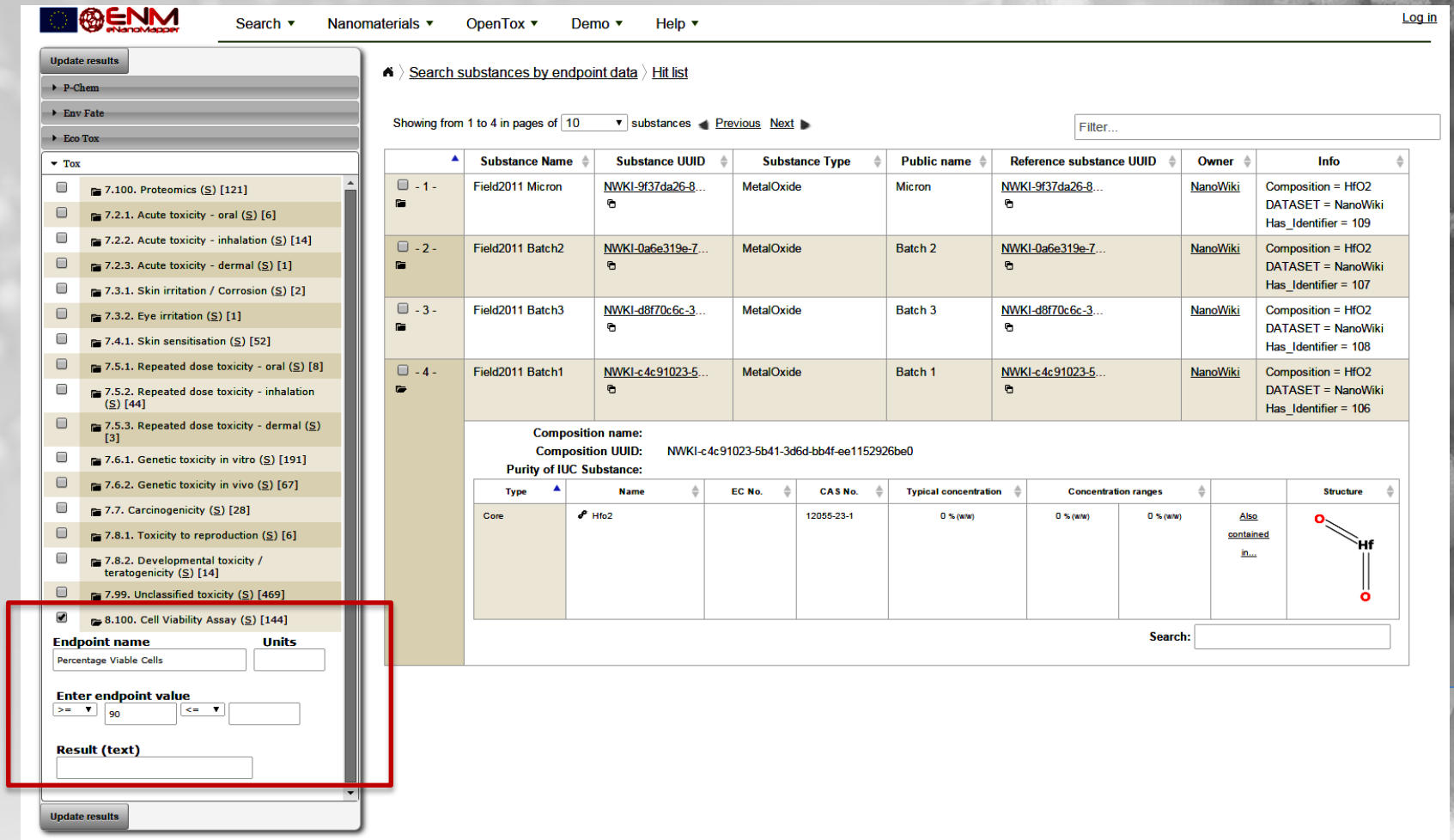
NM toxicity (numeric)



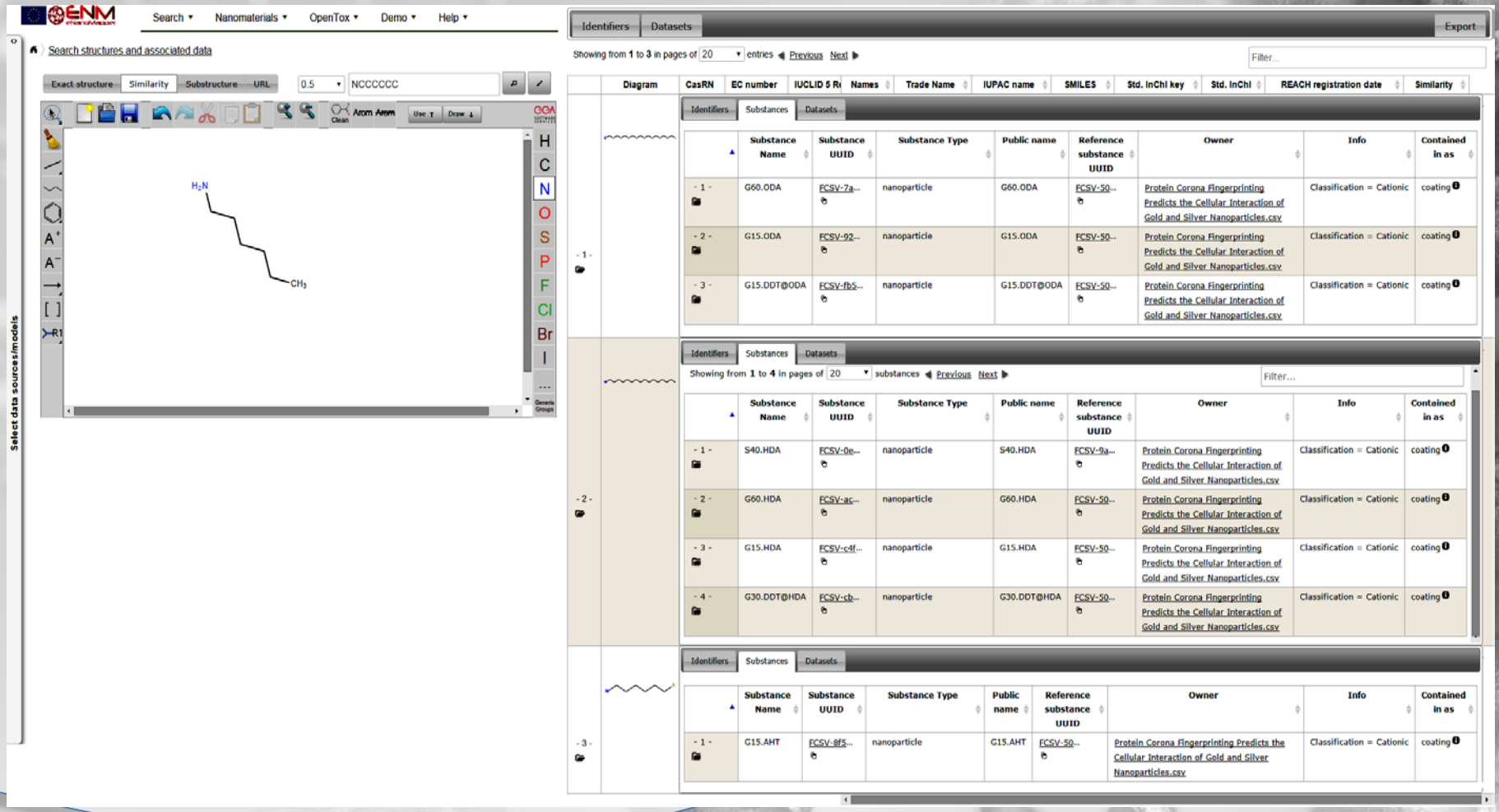
Search by particle size



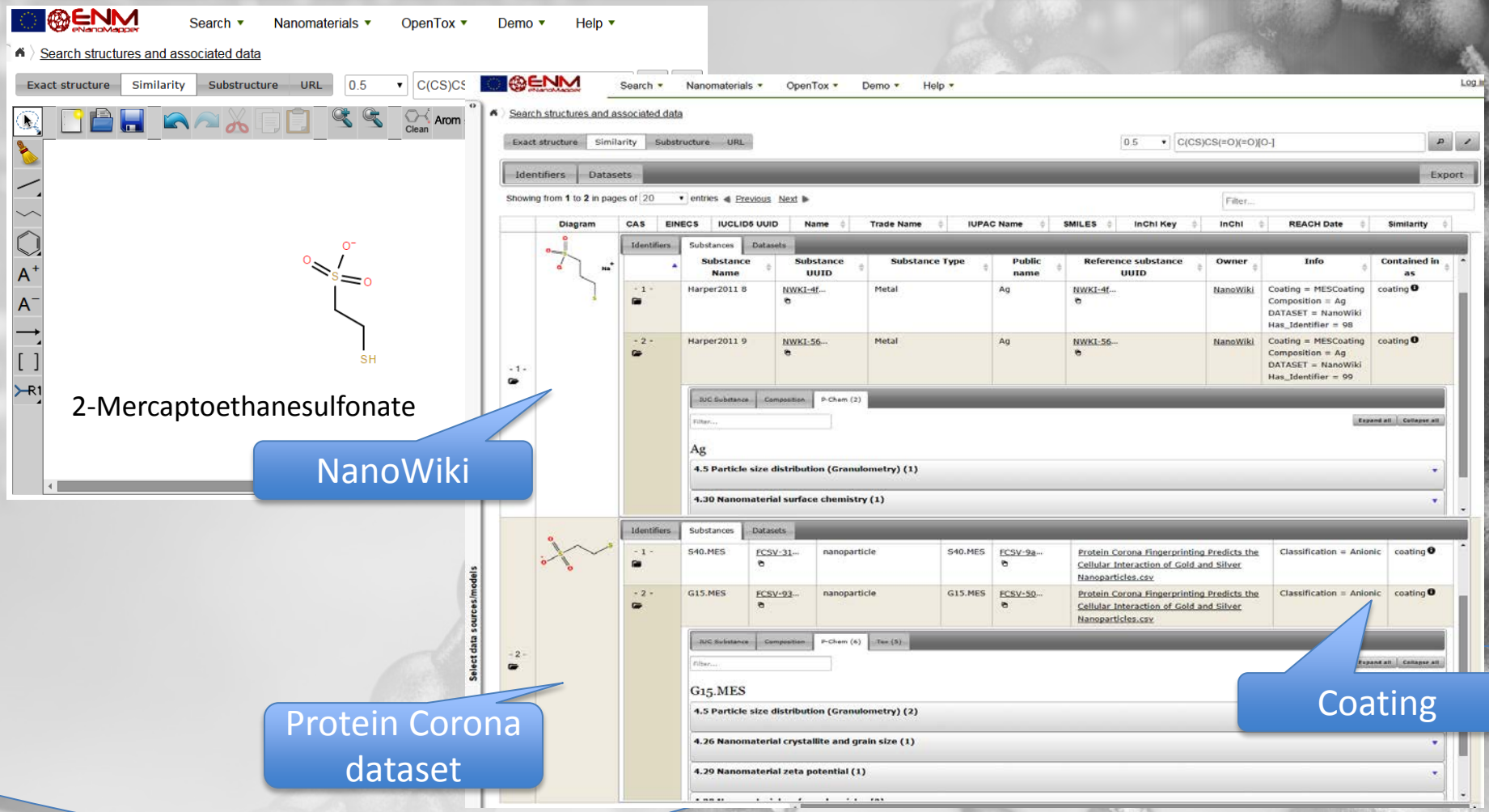
Endpoint search (tox & pchem)



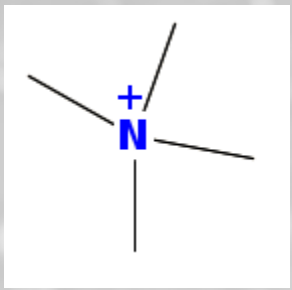
Chemical similarity search



Chemical similarity search (MES coating)



Chemical substructure search



Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾ Log

Search structures and associated data

Exact structure | Similarity | Substructure | URL

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

Identifiers | Datasets | Export

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

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

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

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

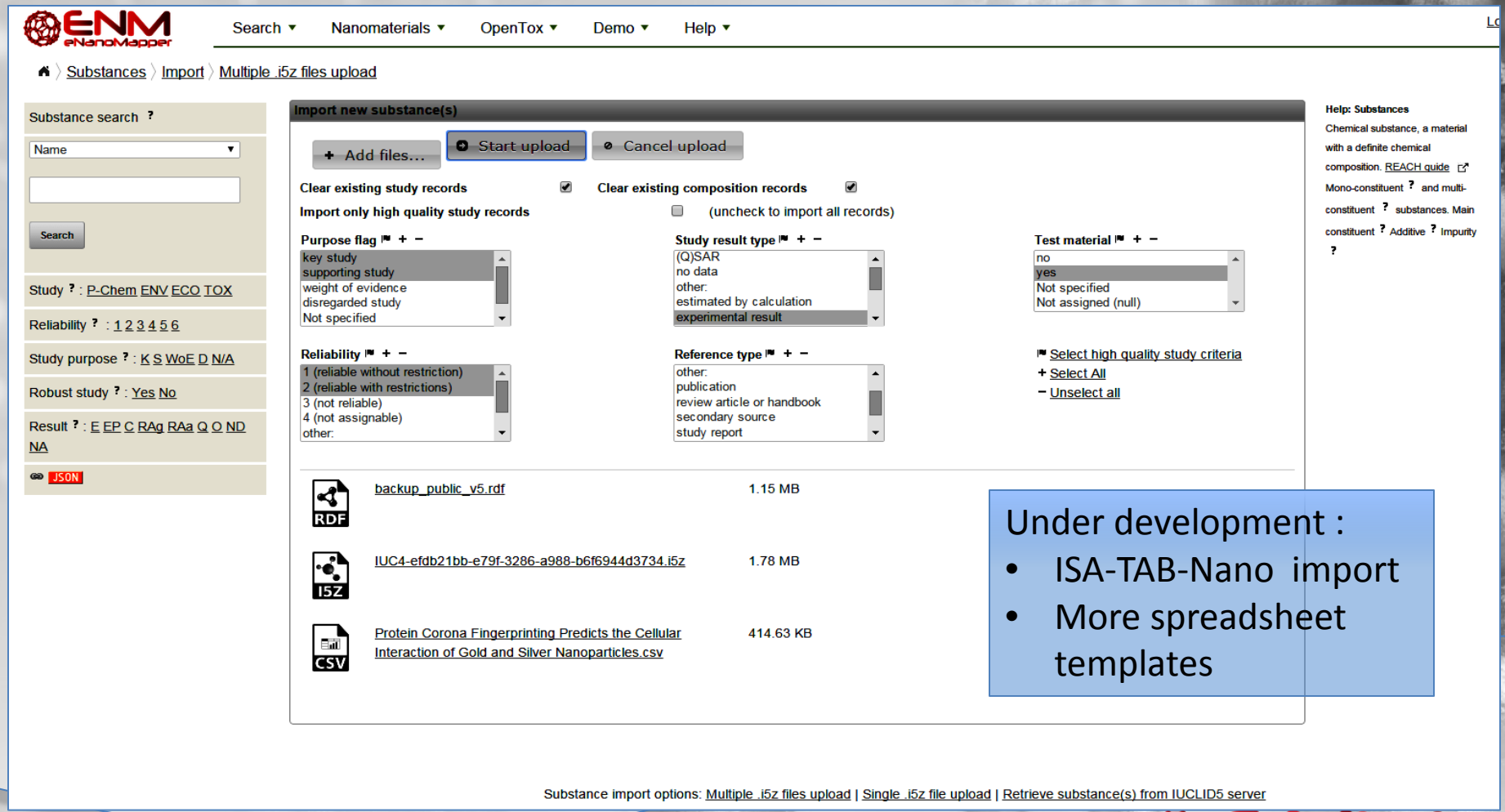
Identifiers | Substances

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

Protein Corona dataset

NanoWiki

Data upload

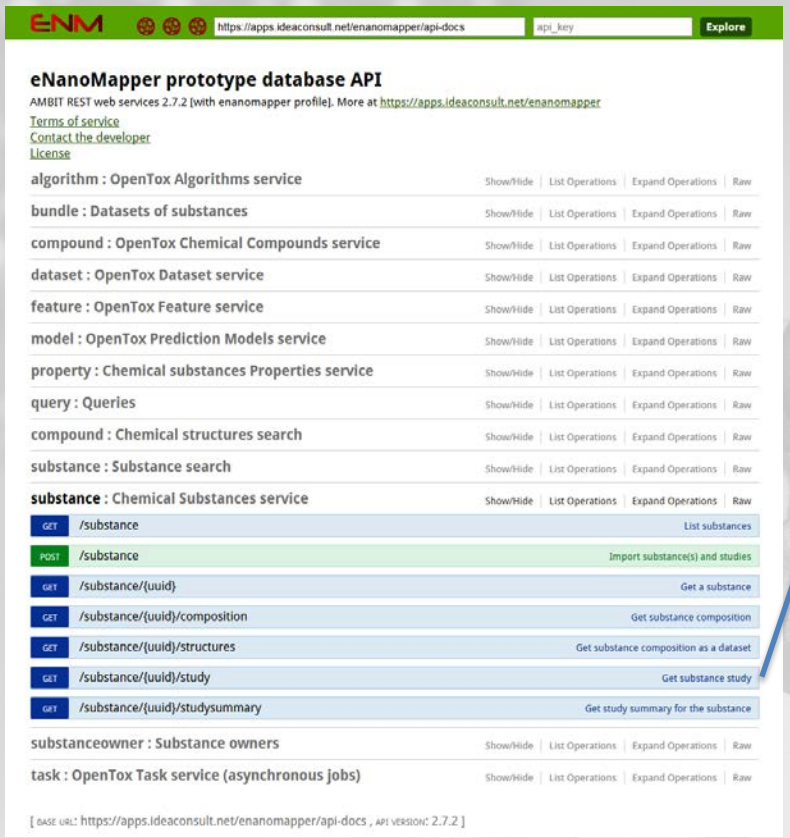


Under development :

- ISA-TAB-Nano import
- More spreadsheet templates

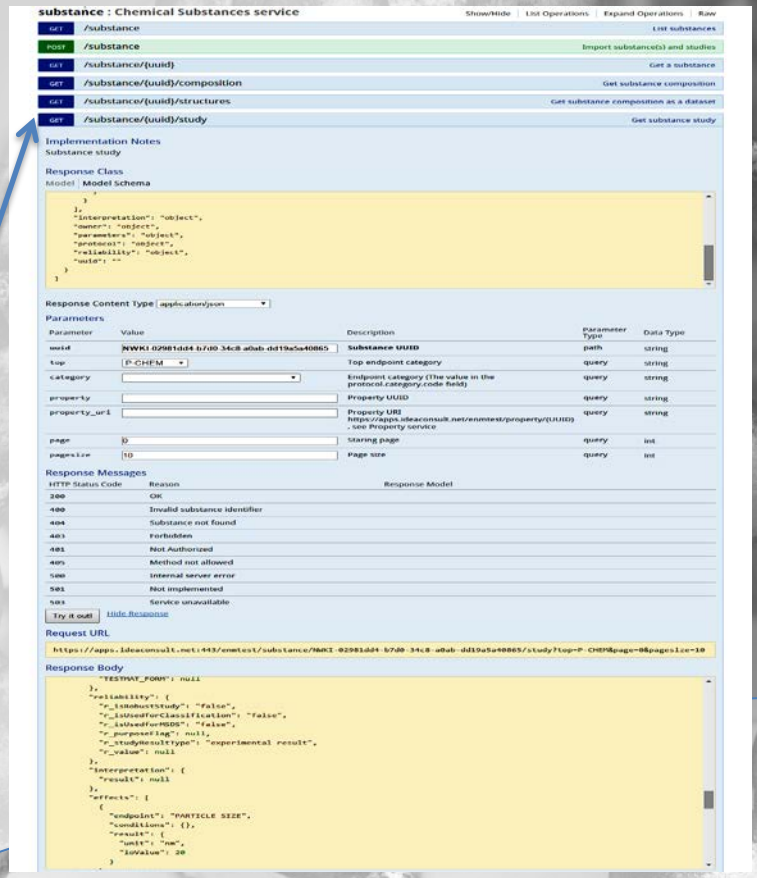
REST Application Programming Interface

API documentation (Swagger-UI)



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

Interactive API queries

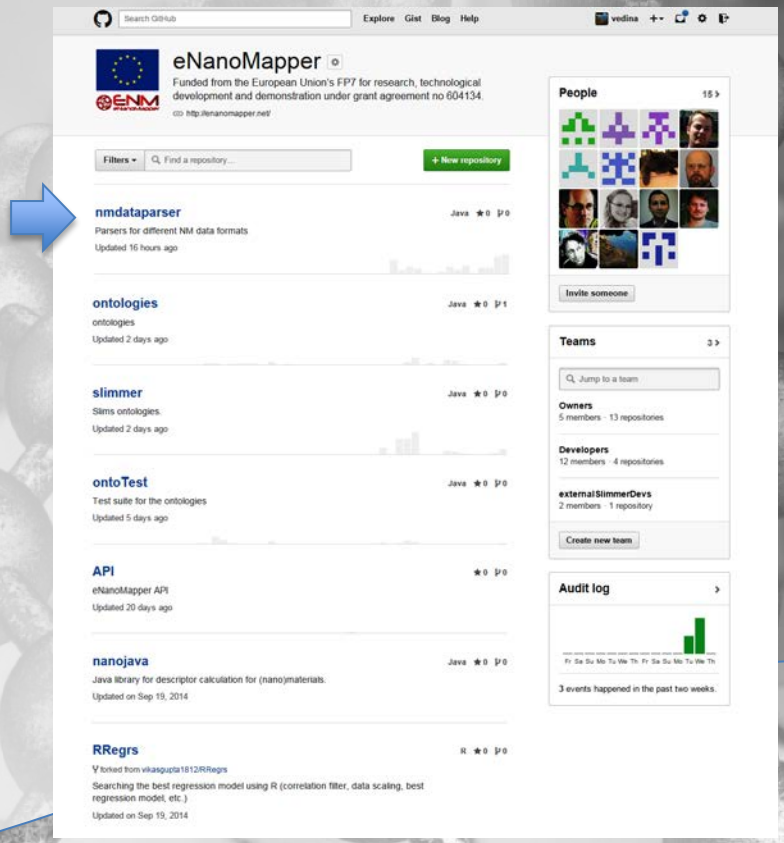


Data formats

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

eNanoMapper@gitHub



Data formats

enanomapper / nmdataparser

Unwatch 15 | Star 0

branch: master

nmdataparser / src / test / resources / net / enanomapper / parser / csv / **ProteinCoronaTest1.json**

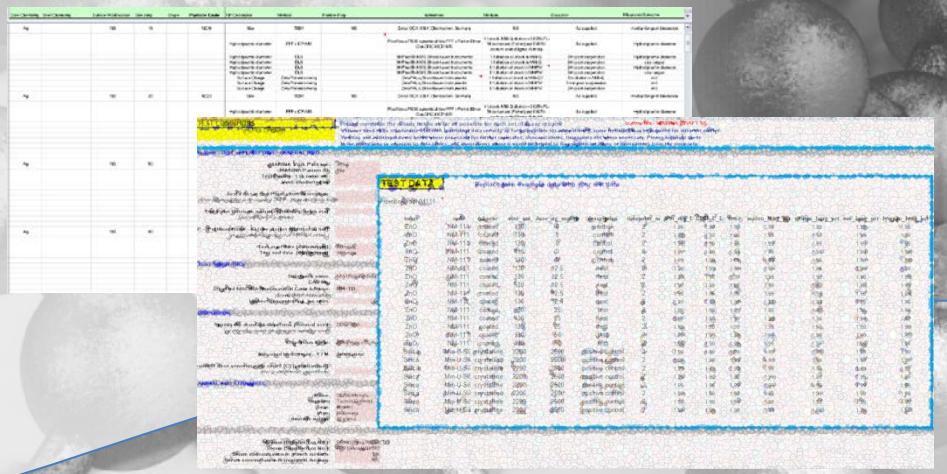
214 lines (214 sloc) | 7.107 kb

Raw | Blame | History

```
{
    "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": {
            "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",
```

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 composi	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															
5	type_of_method				ICP-AES					TEM		TEM				DLS
6	data_gathering_instru	Description			Perkin-Elmer					Tecnai 20		Tecnai 20 (FEI) microscope;AMT 16000 car				ZetaSizer
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				A549	A549	A549	A549	A549							
9	MEDIUM															
10	Condition															
11	Designation				Mean	SD	N	Mean	Std	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	30.95



eNanoMapper

Questions?

THANK YOU!

eNM
eNanoMapper