

The first eNanoMapper prototype: a substance database to support safe-by-design

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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

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
- 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.

Q: Why no common DB approach?

Answer: Because it is hard



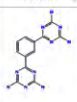




- Getting the data model right is hard
- Making the data model universal is hard
- Reasons:
 - Material
 - Uniqueness
 - Experimental data
 - Complexity
 - Modelling
 - Different requirements

Analogy: Chemical structures DB

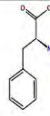

- Chemical structure and Properties
- Data model not appropriate. Instead:
 - Substances - measured properties
 - Structure - calculated properties.
- Substances composition
 - Constituents, impurities, additives
- Nanomaterials
 - Core, coating(s), linkage
 - Also impurities

Substance, Material, Composition

Substance (formaldehyde)

Substance Name	Substance UID	Substance Type	Public name	Reference substance UID	Owner	Info
formaldehyde (IUC4 DSN 52)	IUC4-efdb21bb-e7	Existing Chemical		ECB5-053aa8c4-d	OECD / Paris / France	IUCID4 = DSN 52
Composition name: Other: Pure Composition UID: L340667b-e95f-3743-6236-1b9b25a94d56 Purity of IUC Substance: 0.0 % (w/w)						
Type	Name	EC No.	CAS No.	Typical concentration	Concentration ranges	Structure
Constituent	Formaldehyde	200-001-6	50-00-0	100 % (w/w)	0 % (w/w) - 0 % (w/w)	Also contained in... 
Composition name: Other: Sales Products In Aqueous Solution Composition UID: L-c1f007214067-37fd-a233-e9a2463c-4d3c Purity of IUC Substance:						
Type	Name	EC No.	CAS No.	Typical concentration	Concentration ranges	Structure
Constituent	Formaldehyde	200-001-6	50-00-0	0 % (w/w)	0 % (w/w) - 0 % (w/w)	Also contained in... 
Composition name: Composition UID: L-Q2d3bc-7e-a154-3f6d-babb-22ea28467466 Purity of IUC Substance:						
Type	Name	EC No.	CAS No.	Typical concentration	Concentration ranges	Structure
Active	6-[2-(4-8-oxocanyloxy)-1,3,5-Triazo-2-yl]Phenyl-1,3,5-Triazine-2,4-Diazine-5,6-dithioazolo-... UHffccayce: N:100014011261211010113-6: 17-716100140114011-09-0-1-3-04: 58-19-1111020-1216102411-46-14-13-14-17-18-21)	225-859-0	5118-80-0	0 % (w/w)	0 % (w/w) - 0 % (w/w)	Also contained in... 
Active (solvent)	Water	231-791-2	7732-18-5	ca 40 % (w/w)	0 % (w/w) - 0 % (w/w)	Also contained in... 
Impurity	Formic Acid	200-076-1	64-18-0	ca 0.3 % (w/w)	0 % (w/w) - 0 % (w/w)	Also contained in... 
Impurity	Iron(Iso[2+])	231-094-4	7439-89-6	ca 0.0001 % (w/w)	0 % (w/w) - 0 % (w/w)	Also contained in... 
Impurity	Methanol	200-656-6	67-68-1	0 % (w/w)	0.5 % (w/w) - 2 % (w/w)	Also contained in... 

Gold Nanoparticle

Substance Name	Substance UID	Substance Type	Public name	Reference substance UID	Owner	Info
G15.Phe	FCSV-43f0ea59-a...	nanoparticle	G15.Phe	FCSV-50cca421-d...	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Anionic
Composition name: Composition UID: FCSV-43f0ea59-aa2f-31d8-8d87-19c95ec9be18 Purity of IUC Substance:						
Type	Name	EC No.	CAS No.	Typical concentration	Concentration ranges	Structure
Coating	(2s)-2-Azanylo-3-Phenylpropanoic Acid Colvinthylwikis-Ommngobosa-N,Indin1sC6h11no2C10-8(11)12(6-7-4-2-1-3-6-7)H1-5,8h,8,10h2(4-11,12)T8-IMQSI (2s)-2-Amino-3-Phenylpropanoic Acid (2s)-2-Amino-3-Phenylpropanoic Acid (2s)-2-Amino-3-Phenylpropanoic Acid L-Phenylalanine			0 % (w/w)	0 % (w/w) - 0 % (w/w)	Also contained in... 
Core	[Au]			0 % (w/w)	0 % (w/w) - 0 % (w/w)	Also contained in... 

Experimental data

- **Typical assay description**
 - Property – value (range of values) – units (*Excel templates*)
- **More complex description:**
 - Experimental graph (*ISA-TAB / ISA-TAB-nano*)
- **Commonalities:**
(*BioAssay Ontology, OECD Harmonized Templates, CoDATA UDS*)
 - Materials sample
 - Protocols, protocol parameters, experimental conditions
 - Readouts
 - Measurements, Measurement groups, Raw data, derived data

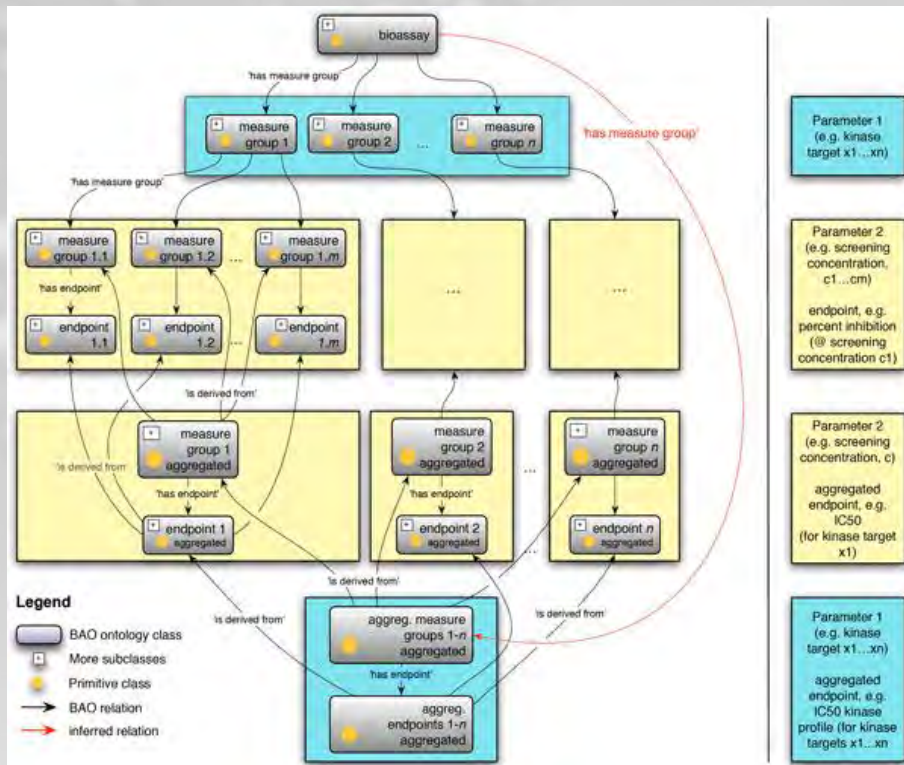
OECD Harmonized Templates (<http://iuclid.eu>)

The screenshot displays the IUCLID software interface. On the left is a navigation tree with a red box highlighting the '4 Physical and chemical properties' section, specifically '4.24 Agglomeration/aggregation' and its sub-item 'Agglomeration/aggregation.001'. The main window shows the 'Endpoint study record' for 'Agglomeration/aggregation.001'. The 'Results and discussions' section is active, showing several data entry fields: 'Agglomerate/Aggregate diameter' (Mean diameter: 33, St. Deviation: 5, pH: 9, Medium: xxx), 'Agglomerate/Aggregate size' (Percentile: D50, Mean: 33, St. Deviation: 5, pH:), 'Agglomerate/Aggregate size distribution at different conditions' (Seq. Num., Size, Distribution, Remarks), and 'Agglomeration/Aggregation Index' (Mean, pH, Medium, Remarks). The bottom of the window has a section for 'Overall remarks, attachments'.

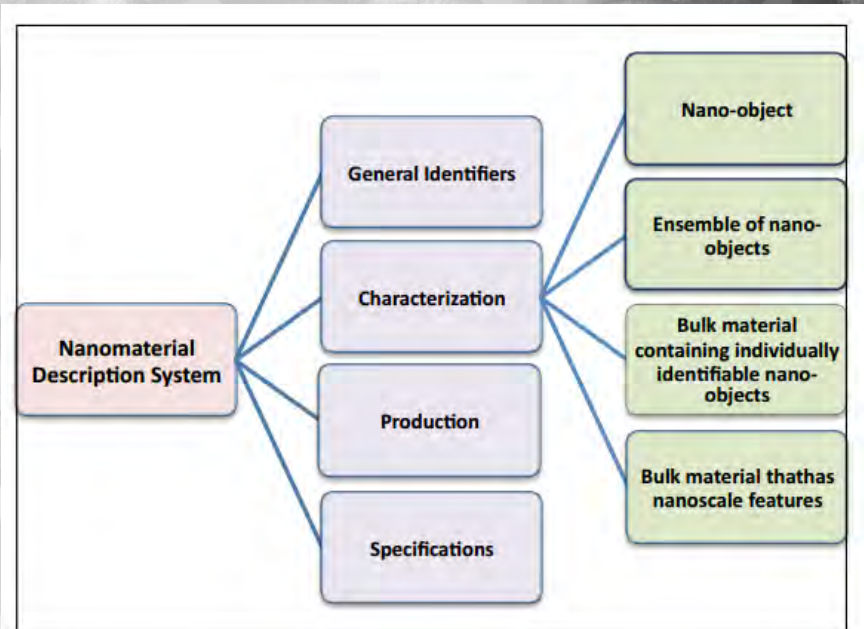
- ... 4.24 Agglomeration/aggregation
 - **Agglomeration/aggregation.001**
- + ... 4.25 Crystalline phase
- + ... 4.26 Crystallite and grain size
- + ... 4.27 Aspect ratio/shape
- + ... 4.28 Specific surface area
- + ... 4.29 Zeta potential
- + ... 4.30 Surface chemistry
- + ... 4.31 Dustiness
- + ...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

More data models

BioAssay Ontology



CODATA Uniform Description System for Materials at the Nanoscale



What we need to describe NM and related experiments

What we need to describe a nanomaterial and related experiments

- **A.** An ontology describing a nanoparticle and a part of the manufacturing process. A file (e.g. `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.1.** Sample level specific to the experiment - defined in `m_*.file`
- **B.2.** ISA - 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 [L25](#))
- **B.3.** The nanomaterial will be linked to the chemical groups where relevant (e.g. silver nanoparticle - linked to Ag - as in [OpenToxic Compounds API](#))

Unique identifier
Substance / Material
(composition, linkage)

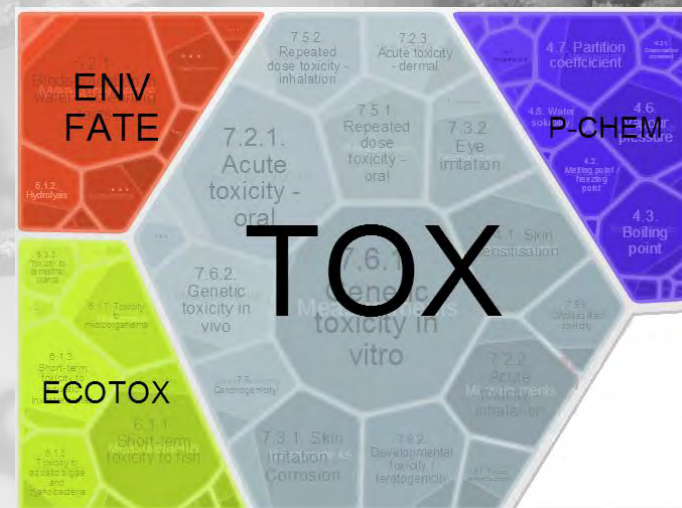
- **C.** Attach measurements to **B**. A *measurement* is defined by applying a protocol **P** (with certain parameters) to the sample **B**. The experimental design might include several sets of conditions/factors (e.g. species, concentrations, etc.) and one or more readouts (results). The parameters, 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
- Do all measurements - grouped by material, protocol, protocol?

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

[data.enanomapper.net](https://apps.ideaconsult.net/enanomapper/ui)

The screenshot shows a web browser window with the URL <https://apps.ideaconsult.net/enanomapper/ui>. The page features a navigation menu with 'Search', 'Nanomaterials', 'OpenTox', 'Demo', and 'Help'. The main heading is 'Welcome to eNanoMapper prototype database', with a subtitle 'A substance database to support safe-by-design engineered nano materials'. Below this is a 'Simple search' section with a text input field containing '[Au]' and a 'Search' button. At the bottom, there are logos for 'OpenTox', 'ENM eNanoMapper', 'SEVENTH FRAMEWORK PROGRAMME', and the European Union flag.



2014-11-02

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

Nanomaterials overview



Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

Lo

Home / [Admin](#) / [Statistics](#) / [Substances per owner](#)

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](#) [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 ?](#)

Showing 1 to 4 of 4 entries

First Previous 1 Next Last

Substance contributor Name ▲	Substances ◆	Table view ◆	Substance contributor UUID ◆
Ideaconsult Ltd. / Sofia / Bulgaria	Substances [1]	Substances and data Chemical structures	IUC5-354430C7-746E-450E-9722-09788EB90A29
NanoWiki	Substances [330]	Substances and data Chemical structures	NWKI-9F4E86D0-C85D-3E83-8249-A856659087DA
OECD / Paris / France	Substances [1]	Substances and data Chemical structures	IUC4-44BF02D8-47C5-385D-B203-9A8F315911CB
Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Substances [121]	Substances and data Chemical structures	FCSV-319611C6-E7DA-3977-A5AC-EB74D49A4319

Show

10 ▾

entries

Filter:

Protein Corona Data set

ENM eNanoMapper Search Nanomaterials OpenTox Demo Help

Search substances by identifiers

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

Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info
G15.DDT@BDHDA	ECSV-2a853f39-4...	nanoparticle	G15.DDT@BDHDA	ECSV-2a853f39-4...	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic
G15.DDT@CTAB	ECSV-d1731b11-2...	nanoparticle	G15.DDT@CTAB	ECSV-d1731b11-2...	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic
G15.DDT@DOTAP	ECSV-3b96ad7a-b...	nanoparticle	G15.DDT@DOTAP	ECSV-3b96ad7a-b...	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic
G15.DDT@ODA	ECSV-fb5e6048-8...	nanoparticle	G15.DDT@ODA	ECSV-fb5e6048-8...	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic

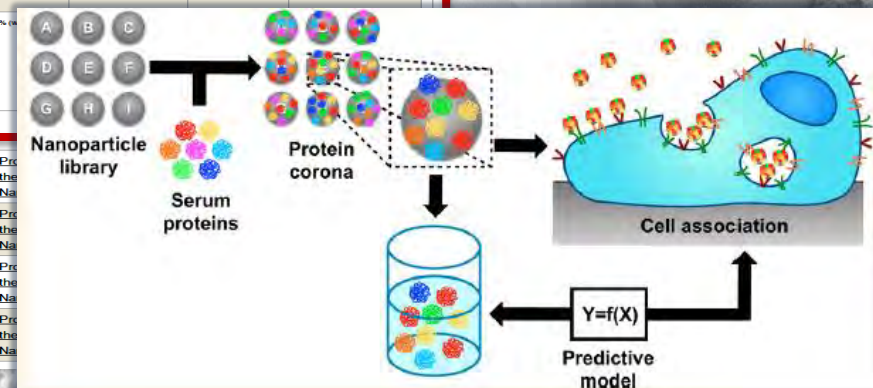
Composition name: FCSV-fb5e6048-8ee1-351d-915b-d1669681357e

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.Wnahlzmdsqwpp-Uhfffaoya-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)	Also contained in...	
Coating	Octadecan-1-Amine.Rxyjpsvuyrzge-Uhfffaoya-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,1-Octadecylamine			0 % (w/w)	0 % (w/w)	Also contained in...	
Core	[Au]			0 % (w/w)	0 % (w/w)		

G15.DDT@SA	ECSV-cd7105f2-f...	nanoparticle	G15.DDT@SA	ECSV-cd7105f2-f...	Pro the Na	
G15.DDT@SDS	ECSV-9505d90b-f...	nanoparticle	G15.DDT@SDS	ECSV-9505d90b-f...	Pro the Na	
G30.DDT@BDHDA	ECSV-50aee96c-a...	nanoparticle	G30.DDT@BDHDA	ECSV-50aee96c-a...	Pro the Na	
G30.DDT@CTAB	ECSV-c4e9df58-f...	nanoparticle	G30.DDT@CTAB	ECSV-c4e9df58-f...	Pro the Na	



NanoWiki NM



Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

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 Q 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 ?

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 M80	NWKI-00e60625-9...	CarbonNanotube	84	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
- 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

NM components



Search ▾

Nanomaterials ▾

OpenTox ▾

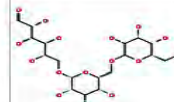
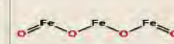
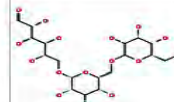
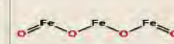
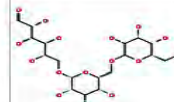
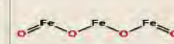
Demo ▾

Help ▾

🏠 Search substances by identifiers

Showing from 1 to 37 in pages of 500 substances ◀ Previous Next ▶

Filter...

Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info																									
Shaw51 45	NWKI-02981ddd4-b...	MetalOxide	MION-47 no. 35	NWKI-02981ddd4-b...	NanoWiki	Alternative Identifier = NP45 Coating = DextranCoating Composition = Fe3O4 DATASET = NanoWiki Has_Identifier = 75																									
<p>Composition name: Composition UUID: NWKI-02981ddd4-b7d0-34c8-a0ab-dd19a5a40865 Purity of IUC Substance:</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>Structure</th> </tr> </thead> <tbody> <tr> <td>Coating</td> <td> <p>☞ (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.FzwbhmxjmoXu-Blaupyhosa-N, Inchi=1s/C 18h32o16/C 19-1-5(21)9(23)10(24)9(22)9-31-17-16(30)14(28)12(26)8(34-17)4-32-18-15(29)13(27)11(25)7(2-20)33-18/H 1,5-18,20-30h,2-4h2/T5-.6+7+,8+,9+,10+,11+,12+,13-,14-,15+,16+,17-,18-M/D/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</p> </td> <td>215-169-8</td> <td>1309-38-2,1317-61-9</td> <td>0 % (w/w)</td> <td>0 % (w/w)</td> <td>0 % (w/w)</td> <td> <p>Also contained in...</p>  </td> </tr> <tr> <td>Core</td> <td>☞ Magnetite, Fe3o4</td> <td>215-169-8</td> <td>1309-38-2,1317-61-9</td> <td>0 % (w/w)</td> <td>0 % (w/w)</td> <td>0 % (w/w)</td> <td> <p>Also contained in...</p>  </td> </tr> </tbody> </table>							Type	Name	EC No.	CAS No.	Typical concentration	Concentration ranges			Structure	Coating	<p>☞ (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.FzwbhmxjmoXu-Blaupyhosa-N, Inchi=1s/C 18h32o16/C 19-1-5(21)9(23)10(24)9(22)9-31-17-16(30)14(28)12(26)8(34-17)4-32-18-15(29)13(27)11(25)7(2-20)33-18/H 1,5-18,20-30h,2-4h2/T5-.6+7+,8+,9+,10+,11+,12+,13-,14-,15+,16+,17-,18-M/D/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</p>	215-169-8	1309-38-2,1317-61-9	0 % (w/w)	0 % (w/w)	0 % (w/w)	<p>Also contained in...</p> 	Core	☞ Magnetite, Fe3o4	215-169-8	1309-38-2,1317-61-9	0 % (w/w)	0 % (w/w)	0 % (w/w)	<p>Also contained in...</p> 
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Core	☞ Magnetite, Fe3o4	215-169-8	1309-38-2,1317-61-9	0 % (w/w)	0 % (w/w)	0 % (w/w)	<p>Also contained in...</p> 																								

NM Phys chem



Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

LOC

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 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 (4)
Tox (5)

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 nm	DOI	DLS	DLS	-	NWKI-2433959f-8955-48b0-...
-	-	-	PARTICLE SIZE	= 221 nm	DOI		-	-	NWKI-bc3b5b48-5780-401e-...

Showing 2 study(s) (1 to 2)

◀ Previous Next ▶

4.29 Nanomaterial zeta potential (2)

Type of meth	Endpoint	Test Mater Form	Result	Remarks	pH	Medium	Reference	Guideline	Owner	UUID
-	ZETA POTENTIAL	-	= 64 mV	-	-	-	DOI		-	NWKI-a2561ddb-9dc8-4190-...
-	ZETA POTENTIAL	-	= 64 mV	-	-	-	DOI		-	NWKI-abe3b28d-9b2a-4c8d-...

Showing 2 study(s) (1 to 2)

◀ Previous Next ▶

NM toxicity (classifier)



Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

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

Filter...

Expand all Collapse all

CuO

8.100 Cell Viability Assay (9)

Reference	Cell line	Doses/concentrations	Endpoint	Result	Result (text)	Guideline	Owner	UUID
2011	BEAS-2B	= 1 mg/L	Toxicity Classifier	-	Non-toxic		Small	NWKI-64c2f9f2-15fc-4406-a... 🗑️
2011	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)



Home > 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

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	Res (text)	Guid	Owner	UUID
2011	HaCaT	= 10 mg/L	Percentage Viable Cells	= 101	-		Chemosphere	NWKI-1bcd287a-291e-4173-...
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-...
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-...

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

Search by particle size

ENM eNanoMapper Search Nanomaterials OpenTox Demo Help

Search substances by endpoint data Hit list

Update results

P-Chem

- 4.1. Appearance (2) [3]
- 4.2. Melting point / freezing point (1) [3]
- 4.26. Nanomaterial crystallite and grain size (105) [105]
- 4.27. Nanomaterial aspect ratio/shape (2) [3]
- 4.28. Nanomaterial specific surface area (8) [8]
- 4.29. Nanomaterial zeta potential (230) [248]
- 4.3. Boiling point (1) [5]
- 4.30. Nanomaterial surface chemistry (183) [367]
- 4.31. Nanomaterial dustiness (1) [1]
- 4.5. Particle size distribution (Granulometry) (356) [496]
- 4.6. Vapour pressure (1) [4]
- 4.7. Partition coefficient (1) [3]
- 4.8. Water solubility (1) [4]

Endpoint name: PARTICLE SIZE Units: nm

Value: >= 55 <= 60

Update results

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

	Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info
- 1 -	Cytotox2011Pyzun14	NWKI-134adc08-a...	MetalOxide	CoO2	NWKI-134adc08-a...	NanoWiki	Composition = CoO2 DATASET = NanoWiki Has_Identifier = 14
- 2 -	Cytotox2011Puzyn09	NWKI-e6ef5597-a...	MetalOxide	Fe2O3	NWKI-e6ef5597-a...	NanoWiki	Composition = Fe2O3 DATASET = NanoWiki Has_Identifier = 9
- 3 -	Cytotox2011Pyzun13	NWKI-81b5a54c-5...	MetalOxide	TiO2	NWKI-81b5a54c-5...	NanoWiki	Composition = TiO2 DATASET = NanoWiki Has_Identifier = 13
- 4 -	Cytotox2011Puzyn08	NWKI-a33b26f0-2f...	MetalOxide	Al2O3	NWKI-a33b26f0-2f...	NanoWiki	Composition = Al2O3 DATASET = NanoWiki Has_Identifier = 1
- 5 -	Cytotox2011Pyzun12	NWKI-f053b420-8...	MetalOxide	SnO2	NWKI-f053b420-8...	NanoWiki	Composition = SnO2 DATASET = NanoWiki Has_Identifier = 12
- 6 -	Cytotox2011Pyzun11	NWKI-33c4d0ef-d...	MetalOxide	ZrO2	NWKI-33c4d0ef-d...	NanoWiki	Composition = ZrO2 DATASET = NanoWiki Has_Identifier = 11
- 7 -	Wang2009 NM3	NWKI-205a198f-fc...	MetalOxide	Nano-Al2O3	NWKI-205a198f-fc...	NanoWiki	Composition = Al2O3 DATASET = NanoWiki Has_Identifier = 166
- 8 -	Cytotox2011Puzyn07	NWKI-f40bf8a-12...	MetalOxide	Sb2O3	NWKI-f40bf8a-12...	NanoWiki	Composition = Sb2O3 DATASET = NanoWiki Has_Identifier = 8
- 9 -	Cytotox2011Puzyn10	NWKI-845bf8fc-78...	MetalOxide	SiO2	NWKI-845bf8fc-78...	NanoWiki	Composition = SiO2 DATASET = NanoWiki Has_Identifier = 10
- 10 -	Cytotox2011Pyzun17	NWKI-569828c8-e...	MetalOxide	La2O3	NWKI-569828c8-e...	NanoWiki	Composition = La2O3 DATASET = NanoWiki Has_Identifier = 17

Endpoint search (tox & pchem)

ENM eNanoMapper Search Nanomaterials OpenTox Demo Help

Search substances by endpoint data Hit list

Update results

P-Chem

- 4.1. Appearance (2) [3]
- 4.2. Melting point / freezing point (1) [3]
- 4.26. Nanomaterial crystallite and grain size (105) [105]
- 4.27. Nanomaterial aspect ratio/shape (2) [3]
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- 4.7. Partition coefficient (1) [3]
- 4.8. Water solubility (1) [4]

Env Fate

Eco Tox

Tox

Update results

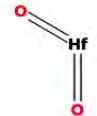
Showing from 1 to 4 in pages of 10 substances Previous Next

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 similarity search

ENM eNanoMapper Search Nanomaterials OpenTox Demo Help

Search structures and associated data

Exact structure Similarity Substructure URL 0.5 Filter...

Diagram

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

Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info	Contained in as
- 1 -	G15.AHT	ECSY-8f5--b	nanoparticle	G15.AHT	ECSY-50--b	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic coating?


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

Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info	Contained in as
- 1 -	G60.ODA	ECSY-7a--b	nanoparticle	G60.ODA	ECSY-50--b	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic coating?
- 2 -	G15.ODA	ECSY-92--b	nanoparticle	G15.ODA	ECSY-50--b	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic coating?
- 3 -	G15.DDT@ODA	ECSY-fb5--b	nanoparticle	G15.DDT@ODA	ECSY-50--b	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

Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info	Contained in as
- 1 -	S40.HDA	ECSY-0b--b	nanoparticle	S40.HDA	ECSY-9a--b	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic coating?
- 2 -	G60.HDA	ECSY-ap--b	nanoparticle	G60.HDA	ECSY-50--b	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic coating?
- 3 -	G15.HDA	ECSY-c4f--b	nanoparticle	G15.HDA	ECSY-50--b	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic coating?
- 4 -	G30.DDT@HDA	ECSY-eb--b	nanoparticle	G30.DDT@HDA	ECSY-50--b	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic coating?

2014-11-02



Chemical substructure search

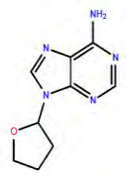
ENM eNanoMapper

Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾


Search structures and associated data

Exact structure ▾ Similarity ▾ Substructure ▾ URL ▾ Custom SMARTS N1C=NC(N)=C2N=CN(C3CCCC3)C=12

Diagram



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

Diagram	CasRN	EC number	IUCLID 5 R	Similarity	IUPAC name	Names	SMILES	REACH registration date	Trade Name
									Coating = CLIO-2DCY35-2DTat Composition = Fe3O4 DATASET = NanoWiki Has_Identifier = 42

Substances

Public Substance: Composition: P-Chem (5)

Filter...

CLIO-Cy5.5-Tat No. 3

4.5 Particle size distribution (Granulometry) (1)

4.29 Nanomaterial zeta potential (1)

4.30 Nanomaterial surface chemistry (3)

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

Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info	Contained in as
Zhang2013 M5	NWKI-13-5	MetalOxide	CoO	NWKI-13-5	NanoWiki	Composition = CoO DATASET = NanoWiki Has_Identifier = 310 SOURCE = Zhang2012	core?

Substances

Public Substance: Composition: P-Chem (1)

Filter...

CoO

4.5 Particle size distribution (Granulometry) (1)

Data upload



Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

Substances > Import > Multiple .i5z 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 RA Q Q ND NA

JSON

Import new substance(s)

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)

Select high quality study criteria
+ Select All
- Unselect all

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

	backup_public_v5.rdf	1.15 MB
	IUC4-efdb21bb-e79f-3286-a988-b6f6944d3734.i5z	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 .i5z files upload](#) | [Single .i5z file upload](#) | [Retrieve substance\(s\) from IUCLID5 server](#)

API

ENM  [Explore](#)

algorithm : OpenTox Algorithms service	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 : 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

eNanoMapper @ github

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



The image shows a complex spreadsheet with multiple columns and rows. A blue border highlights a specific section of the data. There are some yellow and blue highlights on the left side of the spreadsheet, possibly indicating specific rows or columns of interest.

The screenshot shows the GitHub repository page for eNanoMapper. The repository is listed as "eNanoMapper" with a red molecular structure logo. Below the repository name, there is a search bar and a "+ New repository" button. The repository list includes:

- nmdataparser**: Parsers for different NM data formats. Updated a day ago.
- ontologies**: ontologies. Updated 3 days ago.
- ontoTest**: Test suite for the ontologies. Updated 3 days ago.
- slimmer**: Slims ontologies. Updated 3 days ago.
- API**: eNanoMapper API. Updated on Sep 29.
- imageAnalyzer**: Y forked from mkotsianidis/imageAnalyzer. Updated on Sep 26.

On the right side, there is a "People" section with 16 members, a "Teams" section with 3 teams, and an "Audit log" section showing 2 events in the past two weeks.

2014-11-02





www.enanomapper.net/partners

THANK YOU