

NANOREG DATABASE

An instance of the eNanoMapper database and the search application are installed at <https://apps.ideaconsult.net/nanoreg1> and <https://search.data.enanomapper.net/nanoreg>. No registration or login is required since March 20, 2017.

Content

The current content is converted from a SQL dump of the TNO experimental database as provided Jan 23, 2017.

The original NANoREG project data entry was organised in two different ways. Most of the data generated by the NANoREG project is entered via a web entry tool (DET), into a MySQL database, both developed by the Dutch Organization for Applied Scientific Research (TNO). The TNO database design is based on templates developed by the European Joint Research Center (JRC) for assays performed in NANoREG. The TNO database content was converted into eNanoMapper database SQL and this is what is currently available online at the web sites above. Besides the SQL dump, a large amount of NANoREG data is provided as Excel files, provisionally following the NANoREG templates. Cleaning, configuring and importing into the database are ongoing.

Search

Search application with NANOREG data at <https://search.data.enanmapper.net/nanoreg/>

The search application relies on search services and user interface previously reported in eNanoMapper D3.2¹ and D5.5². The search application was considerably updated according to user feedback. A user guide is available at eNanoMapper tutorial repository³.

¹ enanoMapper deliverable D3.2

http://www.enanmapper.net/deliverables/d3/20160420_eNanoMapper_D3.2_Data_Management_System_with_extended_search_capabilities_FINAL.pdf

² eNanoMapper deliverable D5.5

http://www.enanmapper.net/deliverables/d5/20160420_eNanoMapper_D5.5_User_application_for_searching_and_downloading_eNanoMapper_data_FINAL.pdf

³ https://github.com/enanmapper/tutorials/tree/master/Hackathon_on_templates_for_data_collection

2. USER GUIDE

A quick user guide illustrating search and download facilities.

2.1. Go to <https://search.data.enanomapper.net/nanoreg/>

The screenshot shows the NANoREG - eNanoMapper database search interface. The top navigation bar includes links for Home, Search, Data collections, Data templates, and Help. The main header displays the NANoREG logo and the text "NANoREG - eNanoMapper database" and "NANoREG specific license information". A search bar is located on the right. On the left, a sidebar lists various data sources with their respective counts: Data sources (22774), Nanomaterial type (22774), TOX (15574), P-CHEM (7158), ECOTOX (42), Cell (12596), Species (2764), Medium (18216), Dispersion protocol (22536), Experiment year (22774), References (22219), Exposure route (2722), Protocols (22196), and Method (15262). The main content area shows a list of search results under the "Hits list" tab. The results are displayed in a table with columns for "Hits list" and "Selection". The table shows five entries, each with a blue icon, a title, a core description, and a list of results. The first entry is "Ag @ IIT (Ag 20 nm) silver nanoparticle" with results: P-CHEM.Particle size distribution (Granulometry). The second entry is "Au@PBPk (Au 13 nm) gold nanoparticle" with results: P-CHEM.Surface area, P-CHEM.Particle size distribution (Granulometry). The third entry is "CeO2@PBPk (CeO2 140-200 nm) cerium oxide nanoparticle" with results: P-CHEM.Surface area, P-CHEM.Particle size distribution (Granulometry). The fourth entry is "JRCNM01000a(NM-100) (TiO2 50-150 nm) titanium oxide nanoparticle" with results: P-CHEM.Particle size distribution (Granulometry), P-CHEM.Aspect ratio/shape, P-CHEM.Batch Dispersion quality, P-CHEM.Surface area, TOX.Cell Viability, TOX.Immunotoxicity, TOX.Genetic toxicity in vitro, TOX.Repeated dose toxicity - Inhalation. The fifth entry is "JRCNM01001a (NM-101) (TiO2 6 nm) titanium oxide nanoparticle" with results: P-CHEM.Particle size distribution (Granulometry), P-CHEM.Dustiness, P-CHEM.Batch Dispersion quality, P-CHEM.Surface area, P-CHEM.Surface chemistry, TOX.Immunotoxicity, TOX.Genetic toxicity in vitro, TOX.Cell Viability, TOX.Barrier integrity, TOX.Oxidative stress, ECOTOX.Chest term toxicity to aquatic invertebrates, TOX.Repeated dose toxicity - Inhalation, P-CHEM.Zeta potential.

2.2. Enter “carbon nanotube” and Click on “Search” button

This launches the search application you will explore. The page shown in Figure 2 appears.

The screenshot shows the NANoREG - eNanoMapper database search interface. The search query is 'carbon nanotube'. The left sidebar displays a list of data sources (2020) and nanomaterial types (2020). The main panel shows the search results, including a list of hits and a detailed view of the first hit, JRCNM04000a (NM-400) (MWCNT 13.6 nm) carbon nanotube. The detailed view includes the core (1), results (P-CHEM, Particle size distribution (Granulometry), P-CHEM, Batch Dispersion quality, P-CHEM, Dustiness, P-CHEM, Specific surface area, TOX, Immunotoxicity, TOX, Cell Viability, TOX, Genetic toxicity in vitro), and links to Material, Composition, and Studies.

Figure 2 Carbon nanotube search.

There is a search box (top) a summary panel (left) and the results are shown at the main panel. The left panel shows several summaries as shown on Figure 2 .

- Data sources
- Nanomaterial type
- P-Chem
- Tox
- EcoTox
- Medium
- Dispersion protocol
- Results
- References
- Protocols
- Instruments

Every panel is expandable and shows the types of elements found for the particular query, “carbon nanotube” in this case. For example, there are 18 data sources shown, following the NANoREG partners generated data for carbon nanotubes.

2.3. Click on NanoMaterial type at the left

The screenshot shows the NANoREG - eNanoMapper database interface. The search bar at the top contains 'carbon nanotube'. On the left sidebar, the 'Nanomaterial type (2020)' filter is selected, and 'carbon nanotube' is entered in the filter box. The main results area displays a list of four carbon nanotube entries, each with a core ID, name, and a summary of results. The results are filtered to show only carbon nanotubes.

Core ID	Name	Results Summary
JRCNM04000a (NM-400)	(MWCNT 13.6 nm) carbon nanotube	Results: P-CHEM. Particle size distribution (Granulometry), P-CHEM. Batch Dispersion quality, P-CHEM. Dustiness, P-CHEM. Specific surface area, TOX. Immunotoxicity, TOX. Cell Viability, TOX. Genetic toxicity in vitro
JRCNM04001a (NM-401)	(MWCNT 64.2 nm) carbon nanotube	Results: P-CHEM. Particle size distribution (Granulometry), P-CHEM. Batch Dispersion quality, P-CHEM. Dustiness, P-CHEM. Specific surface area, TOX. Immunotoxicity, TOX. Cell Viability, TOX. Genetic toxicity in vitro, TOX. Repeated dose toxicity - oral, P-CHEM. Zeta potential
JRCNM04002a (NM-402)	(MWCNT 12.7 nm) carbon nanotube	Results: P-CHEM. Particle size distribution (Granulometry), P-CHEM. Batch Dispersion quality, P-CHEM. Specific surface area, TOX. Oxidative Stress, TOX. Cell Viability, TOX. Repeated dose toxicity - oral
JRCNM04003a (NM-403)	(MWCNT 12 nm) carbon nanotube	Results: P-CHEM. Batch Dispersion quality, P-CHEM. Particle size distribution (Granulometry), P-CHEM. Specific surface area, TOX. Repeated dose toxicity - oral

Figure 3 The nanomaterial type panel shows carbon nanotube only, because this is what the query is about.

2.4. Click on P-CHEM panel at the left.

P-CHEM stands for physico-chemical characterisation and shows a summary of the type of experiments (the tags marked with green line at the right) and particular parameters measured (the tags marked with blue line at the right).

The screenshot displays the NANoREG - eNanoMapper database search results. The left sidebar contains a list of filters categorized by data sources, nanomaterial types, toxicity (TOX), physico-chemical characterization (P-CHEM), ecotoxicology (ECOTOX), cell studies, species, medium, dispersion protocols, experiment years, references, exposure routes, protocols, and methods. The main search area shows results for 'carbon nanotube' with filters for 'Specific surface area' and 'carbon nanotube'. The results list five entries, each with a core number, a results summary, and links for Material, Composition, and Studies.

Entry	Core	Results Summary	Material	Composition	Studies
JRCNM04000a (NM-400) (MWCNT 13.6 nm) carbon nanotube	JRCNM04000a	Results: P-CHEM. Particle size distribution (Granulometry), P-CHEM. Batch Dispersion quality, P-CHEM. Dustiness, P-CHEM. Specific surface area, TOX. Immunotoxicity, TOX. Cell Viability, TOX. Genetic toxicity in vitro	Material	Composition	Studies
JRCNM04001a (NM-401) (MWCNT 64.2 nm) carbon nanotube	JRCNM04001a	Results: P-CHEM. Particle size distribution (Granulometry), P-CHEM. Batch Dispersion quality, P-CHEM. Dustiness, P-CHEM. Specific surface area, TOX. Immunotoxicity, TOX. Cell Viability, TOX. Genetic toxicity in vitro, TOX. Repeated dose toxicity - oral, P-CHEM. Zeta potential	Material	Composition	Studies
JRCNM04002a (NM-402) (MWCNT 12.7 nm) carbon nanotube	JRCNM04002a	Results: P-CHEM. Particle size distribution (Granulometry), P-CHEM. Batch Dispersion quality, P-CHEM. Specific surface area, TOX. Oxidative Stress, TOX. Cell Viability, TOX. Repeated dose toxicity - oral	Material	Composition	Studies
JRCNM04003a (NM-403) (MWCNT 12 nm) carbon nanotube	JRCNM04003a	Results: P-CHEM. Batch Dispersion quality, P-CHEM. Particle size distribution (Granulometry), P-CHEM. Specific surface area, TOX. Repeated dose toxicity - oral	Material	Composition	Studies
JRCNM40001a (MWCNT 15 nm) carbon nanotube	JRCNM40001a	Results: P-CHEM. Specific surface area, P-CHEM. Particle size distribution (Granulometry)	Material	Composition	Studies
JRCNM40002a (MWCNT 15 nm) carbon nanotube	JRCNM40002a		Material	Composition	Studies

Figure 4 The P-CHEM (physico-chemical characterisation) panel shows the type and the number of entries available for different physicochemical measurements.

Mouse hovering on each tag reveals more information, as number of entries (the colored part of the tag) or ranges of the available measurement (tooltip on the tags marked blue). Clicking a tag adds it to the “current selection” filter (“carbon nanotube” and “specific surface area” shown at Figure 4). The “current selection” can be removed entirely (the button “clear”) or one by one by clicking the corresponding tag. Clicking on “carbon nanotube” tag above the results will remove the filter on CNT and will show all types of materials having data on specific surface area (Figure 5).

The screenshot shows the NANoREG - eNanoMapper database interface. The top navigation bar includes links for Home, Data collections, Data templates, and Help. A search bar is present with the text 'Search' and a 'Feedback' link. The main content area is divided into a left sidebar and a right main panel. The sidebar contains a 'Data sources (16443)' section with a 'Nanomaterial type (16443)' filter and a 'TOX (11680)' filter. The main panel displays a list of nanoparticles, each with a core description, results, and links for more information, material composition, and studies.

Figure 5 All nanomaterials with specific surface area measurements or supplier provided data.

2.6. Click on TOX panel at the left.

TOX stands for toxicity assays, and shows a summary of the type of the experiments (the tags marked with green line at the right) and specific parameters measured (the tags marked with blue line at the right). Any combination of tags can be selected (Figure 6).

The screenshot shows the NANoREG - eNanoMapper database interface. The left sidebar contains a list of filters under 'Data sources (22728)' and 'Nanomaterial type (22728)'. The 'TOX (15567)' filter is selected, and its sub-filters are expanded: 'Repeated dose toxicity - oral', 'Genetic toxicity in vitro', 'Cell Viability', 'Immunotoxicity', 'Barrier integrity', and 'Oxidative Stress'. The main content area displays a 'Hits list' with four entries, each with a 'Selection' tab and an 'Add to Selection' link.

Material	Composition	Studies
Au@PBPBK (Au 13 nm) gold nanoparticle	CORE (1): ...	Results: P-CHEM.Specific surface area, P-CHEM.Particle size distribution (Granulometry)
CeO2@PBPBK (CeO2 140-200 nm) cerium oxide nanoparticle	CORE (1): ...	Results: P-CHEM.Specific surface area, P-CHEM.Particle size distribution (Granulometry)
JRCNM01000a(NM-100) (TiO2 50-150 nm) titanium oxide nanoparticle	CORE (1): ...	Results: P-CHEM.Particle size distribution (Granulometry), P-CHEM.Aspect ratio/shape, P-CHEM.Batch Dispersion quality, P-CHEM.Specific surface area, TOX.Cell Viability, TOX.Immunotoxicity, TOX.Genetic toxicity in vitro, TOX.Repeated dose toxicity - inhalation
JRCNM01001a (NM-101) (TiO2 6 nm) titanium oxide nanoparticle	CORE (1): ...	Results: P-CHEM.Particle size distribution (Granulometry), P-CHEM.Dustiness, P-CHEM.Batch Dispersion quality, P-CHEM.Specific surface area, P-CHEM.Surface chemistry, TOX.Immunotoxicity, TOX.Genetic toxicity in vitro, TOX.Cell Viability, TOX.Barrier integrity, TOX.Oxidative Stress, ECOTOX.Short-term toxicity to aquatic invertebrates, TOX.Repeated dose toxicity - inhalation, P-CHEM.Zeta potential, P-CHEM.Aerosol characterisation
JRCNM01002a(NM-102) (TiO2 21-22 nm) titanium oxide nanoparticle	CORE (1): ...	Results: P-CHEM.Specific surface area, P-CHEM.Particle size distribution (Granulometry)

Figure 6 The current filter includes tags for physicochemical and toxicity assays.

There is “Add to selection” link next to each nanomaterial entry. It allows selecting multiple materials, which will appear in the “Selection” tab. Figure 7 shows the “Selection” tab contains four zinc oxide NM.

The screenshot shows the NANoREG - eNanoMapper database interface with the 'Selection' tab active. The left sidebar shows the 'TOX (15567)' filter selected. The main content area displays a 'Selection (4)' tab with four entries, each with a 'Remove from Selection' link.

Material	Composition	Studies
NM111 (ZnO 141 nm) NPO_1542	CORE (1): ...	Results: P-CHEM.PC_GRANULOMETRY_SECTION, P-CHEM.SPECIFIC_SURFACE_AREA_SECTION, TOX.ENM_0000068_SECTION
NM110 (ZnO 147 nm) NPO_1542	CORE (1): ...	Results: P-CHEM.SURFACE_CHEMISTRY_SECTION, P-CHEM.PC_GRANULOMETRY_SECTION, P-CHEM.ENM_0000081_SECTION, P-CHEM.SPECIFIC_SURFACE_AREA_SECTION, P-CHEM.PC_WATER_SOL_SECTION, TOX.TO_GENETIC_IN_VITRO_SECTION, TOX.ENM_0000044_SECTION, TOX.ENM_0000068_SECTION, TOX.NPO_1339_SECTION, TOX.ENM_0000037_SECTION, ECOTOX.EC_DAPHNIATOX_SECTION, P-CHEM.ZETA_POTENTIAL_SECTION
JRCNM01101a (NM-111) (ZnO 141 nm) NPO_1542	CORE (1): ...	Results: P-CHEM.SURFACE_CHEMISTRY_SECTION, P-CHEM.PC_GRANULOMETRY_SECTION, P-CHEM.ENM_0000081_SECTION, P-CHEM.SPECIFIC_SURFACE_AREA_SECTION, TOX.NPO_1339_SECTION, TOX.ENM_0000068_SECTION, TOX.TO_GENETIC_IN_VITRO_SECTION
JRCNM01100a (NM-110) (ZnO 147 nm) NPO_1542	CORE (1): ...	Results: P-CHEM.SURFACE_CHEMISTRY_SECTION, P-CHEM.PC_GRANULOMETRY_SECTION, P-CHEM.ENM_0000081_SECTION, P-CHEM.SPECIFIC_SURFACE_AREA_SECTION, TOX.TO_GENETIC_IN_VITRO_SECTION, TOX.NPO_1339_SECTION, TOX.ENM_0000068_SECTION, TOX.ENM_0000044_SECTION, P-CHEM.PC_UNKNOWN_SECTION, P-CHEM.ZETA_POTENTIAL_SECTION

Figure 7 The current selection includes tags for physicochemical and toxicity assays.

Since end of Jan 2017, a new tab “Export” is available in the search application, and the query results can be downloaded in different formats. There are several options, defining what to download and in what format.

To download the four selected zinc oxides as Excel file, click on the *XLSX* icon and then click the “Download selected entries as XLSX” (Figure 8).

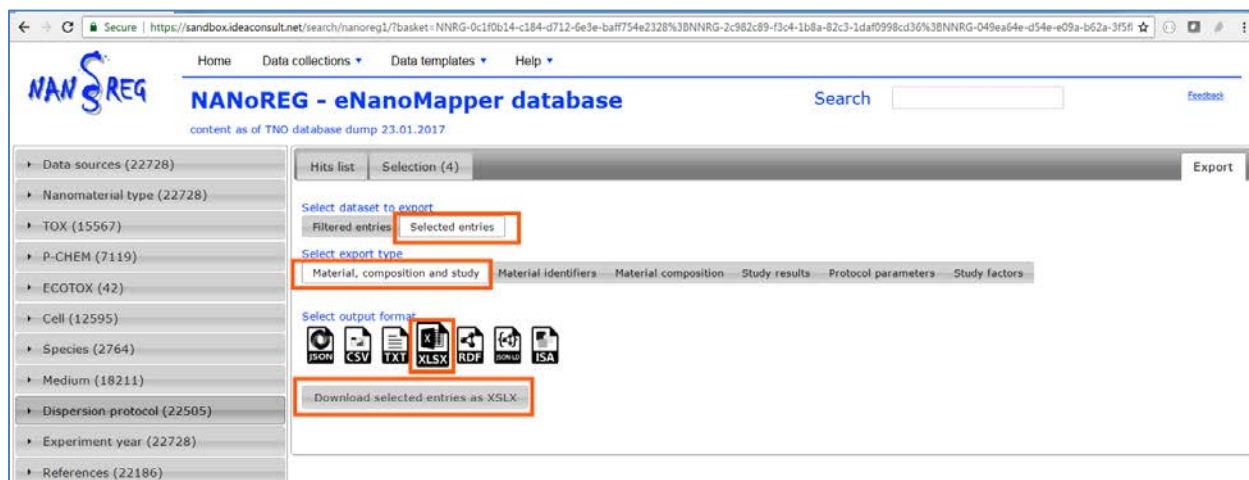


Figure 8 Export selected NM as Excel

To download the search results (NM with surface area and cell viability data, as in Figure 6), specify “Filtered entries”. Click on the XLSX icon. The download button caption will change to “Download filtered entries as XLSX” (Figure 9)

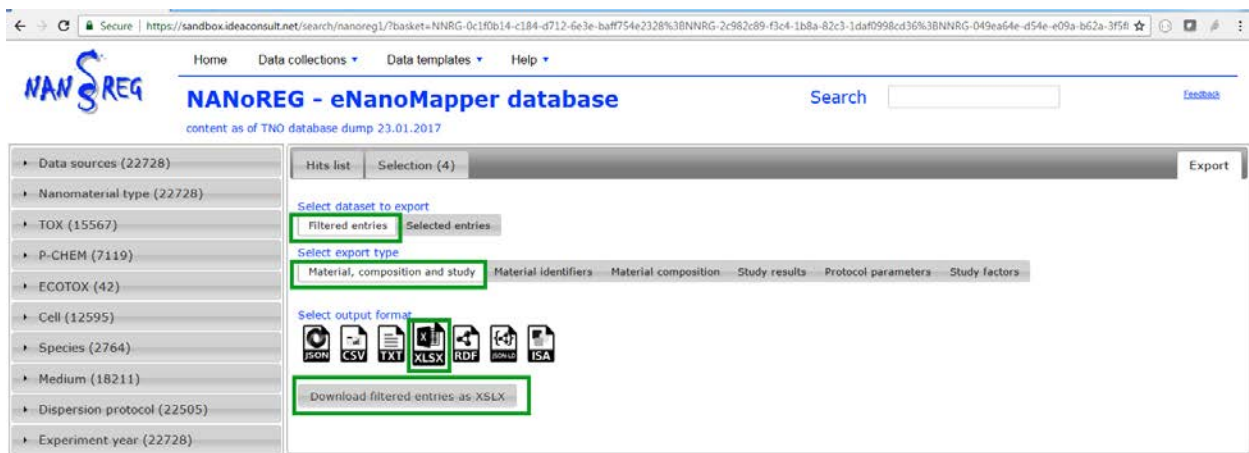


Figure 9 Export search results (filtered entries) as Excel

Please note different *Export type* and the *Output format* combination of options will result in different views of the data (subset of parameters, describing materials and studies). The most

complete view is the JSON ⁴ or RDF ⁵ format with export type "Material, composition and study".

Alternatively, the download facilities of the database application (described in eNanoMapper deliverables D3.2 and D5.5) can be used. For this purpose, follow the links for each material (the *Material/Composition/Study* links at the bottom of each nanomaterial entry). Click on the "Material" link for the NM-100 titanium oxide nanoparticle leads to the database page of the material (Figure 10). There are number of download options.

The screenshot displays the NM-100 nanoparticle database page. At the top, there is a navigation bar with the ENM logo and links for Home, Search, Data collections, Data upload, For developers, and Help. Below this is a search bar with the text "Search nanomaterials by identifiers" and radio buttons for Name, Identifier (selected), Reference, and NM type. The main content area has tabs for "Nanomaterials", "Advanced search", and "Download". Below the tabs, it says "Showing from 1 to 1 in pages of 10 substances" with "Previous" and "Next" links. A table lists the substance details:

Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info
TiO2 50-150 nm	NNRG-18280a4...	NPO_1486	JRCNM01000a(NM-100)		NANoREG	Material code = JRCNM01000a(NM-100) NANoREG material = Core material Supplier = JRC - IHCP, Fraunhofer

Below the table, there is a section for "Composition name: TiO2 Anatase [Impurity Approx 2.3% Wt]" and "Composition UUID: NNRG-18280a4a-45e9-adc0-df3b-125397b1255f". At the bottom, there is a table for "Purity of IUC Substance":

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

Figure 10 The NM-100 nanoparticle database page. The studies are available upon clicks on substance identifiers.

The physicochemical characterisation and bioassay results (Figure 11) are available upon clicks on substance identifiers (e.g. Substance name link)

⁴ JSON (JavaScript Object Notation) <http://www.json.org/>

⁵ https://en.wikipedia.org/wiki/Resource_Description_Framework

The screenshot shows the eNanoMapper web application interface. The main content area displays the search results for the nanoparticle JRCNM01000a(NM-100). The 'P-Chem (38)' tab is selected, showing a list of properties including '4.5 Particle size distribution (Granulometry) (18)', '4.27 Nanomaterial aspect ratio/shape (2)', and '4.28 Nanomaterial specific surface area (2)'. The '4.28 Nanomaterial specific surface area (2)' entry is expanded, showing a table of data:

Reference	Protocol	Endpoint	Result	Owner	Reliability
Provided	Supplier	SPECIFIC SURFACE AREA	9 m ² /g	JRC - IHCP	
Provided	Supplier	SPECIFIC SURFACE AREA	9 m ² /g	Fraunhofer	

Below the table, it indicates 'Showing 2 study(s) (1 to 2)' and provides 'Previous' and 'Next' navigation links. The right sidebar contains links for 'Show structures', 'Remove substance', 'Show substance', and download options for JSON, XML, RDF, and XLSX.

Figure 11 The NM-100 nanoparticle physchem and bioassays database page. The specific surface area entry is expanded, showing supplier provided data.

There are number of download and programmatic access options (API). You may consult the section 3 of the *Search and Download guide*⁶ used in eNanoMapper data workshops for a quick start how to download data from the R statistical package.

3. SUPPORT

- Ask questions at the Ideaconsult collaboration platform <https://phabricator.ideaconsult.net/Q2>
- Or email support@ideaconsult.net

⁶ https://github.com/enanomapper/tutorials/tree/master/Hackathon_on_templates_for_data_collection