

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

NANOREG - eNanoMapper database

content as of TNO database dump 23.01.2017

Home Data collections Data templates Help

Search TiO2 Feedback

Data sources (5337)

Nanomaterial type (5337)

TOX (3525)

P-CHEM (1800)

ECOTOX (12)

Cell (3191)

Species (322)

Medium (4300)

Dispersion protocol (5294)

Experiment year (5337)

References (5137)

Exposure route (310)

Protocols (5027)

Method (3315)

Hits list Selection Export

TiO2

< 1 > displaying 1 to 14 of 14

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

more

Material Composition Studies Add to Selection

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

more

Material Composition Studies Add to Selection

JRCNM01002a(NM-102) (TiO2 21-22 nm) titanium oxide nanoparticle

CORE (1): ...

Results: P-CHEM.Specific surface area, P-CHEM.Particle size distribution (Granulometry)

more

Material Composition Studies Add to Selection

JRCNM01003a(NM-103) (TiO2 24.7 nm) titanium oxide nanoparticle

CORE (1): ...

Results: P-CHEM.Surface chemistry, 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.Genetic toxicity in vitro, P-CHEM.Zeta potential

more

Material Composition Studies Add to Selection

JRCNM01005a (NM-105) (TiO2 23.4 nm) titanium oxide nanoparticle

CORE (1): ...

Results: P-CHEM.Particle size distribution (Granulometry), P-CHEM.Specific surface area

more

Material Composition Studies Add to Selection

JRCNM02003a(NM-203) (TiO2 13-45 nm) titanium oxide nanoparticle

CORE (1): ...

Figure 1 Search application with NANOREG data at <https://search.data.enanomapper.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.enanomapper.net/deliverables/d3/20160420_eNanoMapper_D3.2_Data_Management_System_with_extended_search_capabilities_FINAL.pdf

² eNanoMapper deliverable D5.5

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

³ https://github.com/enanomapper/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 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 "Hits list" with "No filters selected" and "displaying 1 to 20 of 95". It lists five nanoparticles: Ag @ IIT (Ag 20 nm) silver nanoparticle, Au@PBPk (Au 13 nm) gold nanoparticle, CeO2@PBPk (CeO2 140-200 nm) cerium oxide nanoparticle, JRCNM01000a (NM-100) (TiO2 50-150 nm) titanium oxide nanoparticle, and JRCNM01001a (NM-101) (TiO2 6 nm) titanium oxide nanoparticle. Each entry includes a "CORE (1):" link, a "Results:" link, and a "more" link. There are also "Material", "Composition", and "Studies" links for each entry, and an "Add to Selection" button.

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 interface. At the top, there is a search bar with the text 'carbon nanotube' and a 'Search' button. Below the search bar, the database name 'NANoREG - eNanoMapper database' is displayed, along with a note 'content as of TNO database dump 23.01.2017'. On the left side, there is a sidebar with a 'Data sources (2020)' section containing a list of filters: BAUA, CBT, CNR, ENVICAT, FRAUNHOFER, GAIKER, INL, ISQ, JRC - IHCP, KI, LEITAT, NILU, NRCWE, SINTEF, TEKNIKER, TNO, UAB, and UDL. Below this, there is a 'Nanomaterial type (2020)' section with a list of categories: TOX (1498), P-CHEM (522), ECOTOX (42), Cell (715), Species (783), Medium (914), Dispersion protocol (1954), Experiment year (2020), References (1998), Exposure route (783), Protocols (2020), and Method (1498). The main panel on the right shows the search results for 'carbon nanotube'. It includes a 'Hits list' section with a 'Selection' button and an 'Export' button. Below this, there is a list of results, each with a title, a 'CORE (1):' link, and a 'Results:' section. The results are: JRCNM04000a (NM-400) (MWCNT 13.6 nm) carbon nanotube, JRCNM04001a (NM-401) (MWCNT 64.2 nm) carbon nanotube, JRCNM04002a (NM-402) (MWCNT 12.7 nm) carbon nanotube, JRCNM04003a (NM-403) (MWCNT 12 nm) carbon nanotube, and JRCNM40001a (MWCNT 15 nm) carbon nanotube. Each result has a 'Material Composition Studies' link and an 'Add to Selection' button.

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 content area displays a list of search results for 'carbon nanotube', showing 1 to 19 of 19 results. The first four results are visible, each with a blue icon, a title, a core description, and a list of results. The results are: JRCNM04000a (NM-400) (MWCNT 13.6 nm) carbon nanotube, JRCNM04001a (NM-401) (MWCNT 64.2 nm) carbon nanotube, JRCNM04002a (NM-402) (MWCNT 12.7 nm) carbon nanotube, and JRCNM04003a (NM-403) (MWCNT 12 nm) carbon nanotube. Each result has a 'more' link and an 'Add to Selection' button.

NANoREG - eNanoMapper database
content as of TNO database dump 23.01.2017

Search: carbon nanotube

Filter: carbon nanotube

Results: JRCNM04000a (NM-400) (MWCNT 13.6 nm) carbon nanotube
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
more
Material Composition Studies

Results: JRCNM04001a (NM-401) (MWCNT 64.2 nm) carbon nanotube
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, TOX. Repeated dose toxicity - oral, P-CHEM. Zeta potential
more
Material Composition Studies

Results: JRCNM04002a (NM-402) (MWCNT 12.7 nm) carbon nanotube
CORE (1): ...
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
more
Material Composition Studies

Results: JRCNM04003a (NM-403) (MWCNT 12 nm) carbon nanotube
CORE (1): ...
Results: P-CHEM. Batch Dispersion quality, P-CHEM. Particle size distribution (Granulometry), P-CHEM. Specific surface area, TOX. Repeated dose toxicity - oral
more
Material Composition Studies

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 'Filter' section with various categories and their respective entry counts. The main search results area shows a list of entries for 'carbon nanotube' filtered by 'Specific surface area'. The results are displayed in a table-like format with columns for entry ID, name, and a list of results. Each result entry includes a 'CORE (1)' link, a 'Results' section, and links for 'Material', 'Composition', and '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 search results are filtered by 'Specific surface area'. The left sidebar shows various filters including 'Nanomaterial type' and 'TOX'. The main content area displays a list of nanoparticles with their specific surface area measurements and links to detailed information.

Nanomaterial	Specific surface area	Particle size distribution
Au@PBPK (Au 13 nm) gold nanoparticle	Specific surface area, P-CHEM	Particle size distribution (Granulometry)
CeO ₂ @PBPK (CeO ₂ 140-200 nm) cerium oxide nanoparticle	Specific surface area, P-CHEM	Particle size distribution (Granulometry)
JRCNM01000a(NM-100) (TiO ₂ 50-150 nm) titanium oxide nanoparticle	Specific surface area, 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
JRCNM01001a (NM-101) (TiO ₂ 6 nm) titanium oxide nanoparticle	Specific surface area, P-CHEM	Particle size distribution (Granulometry), P-CHEM.Dustiness, P-CHEM.Batch Dispersion quality, 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) (TiO ₂ 21-22 nm) titanium oxide nanoparticle	Specific surface area, P-CHEM	Particle size distribution (Granulometry)

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 icon, a title, a core ID, and a list of results. Each entry has an 'Add to Selection' link.

Selection	Hit	Core ID	Results	Action
☐	Au@PBPk (Au 13 nm) gold nanoparticle	CORE (1): ...	Results: P-CHEM.Specific surface area, P-CHEM.Particle size distribution (Granulometry) more Material Composition Studies	Add to Selection
☐	CeO2@PBPk (CeO2 140-200 nm) cerium oxide nanoparticle	CORE (1): ...	Results: P-CHEM.Specific surface area, P-CHEM.Particle size distribution (Granulometry) more Material Composition Studies	Add to Selection
☐	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 more Material Composition Studies	Add to Selection
☐	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 more Material Composition Studies	Add to Selection
☐	JRCNM01002a(NM-102) (TiO2 21-22 nm) titanium oxide nanoparticle	CORE (1): ...	Results: P-CHEM.Specific surface area, P-CHEM.Particle size distribution (Granulometry) more Material Composition Studies	Add to Selection

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 same filter settings as Figure 6. The main content area displays a 'Selection (4)' list with four entries, each with a selection icon, a title, a core ID, and a list of results. Each entry has a 'Remove from Selection' link.

Selection	Hit	Core ID	Results	Action
☐	NM111 (ZnO 141 nm) NPO_1542	CORE (1): ...	Results: P-CHEM.PC_GRANULOMETRY_SECTION, P-CHEM.SPECIFIC_SURFACE_AREA_SECTION, TOX.ENM_0000068_SECTION more Material Composition Studies	Remove from Selection
☐	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 more Material Composition Studies	Remove from Selection
☐	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 more Material Composition Studies	Remove from Selection
☐	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 more Material Composition Studies	Remove from Selection

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).

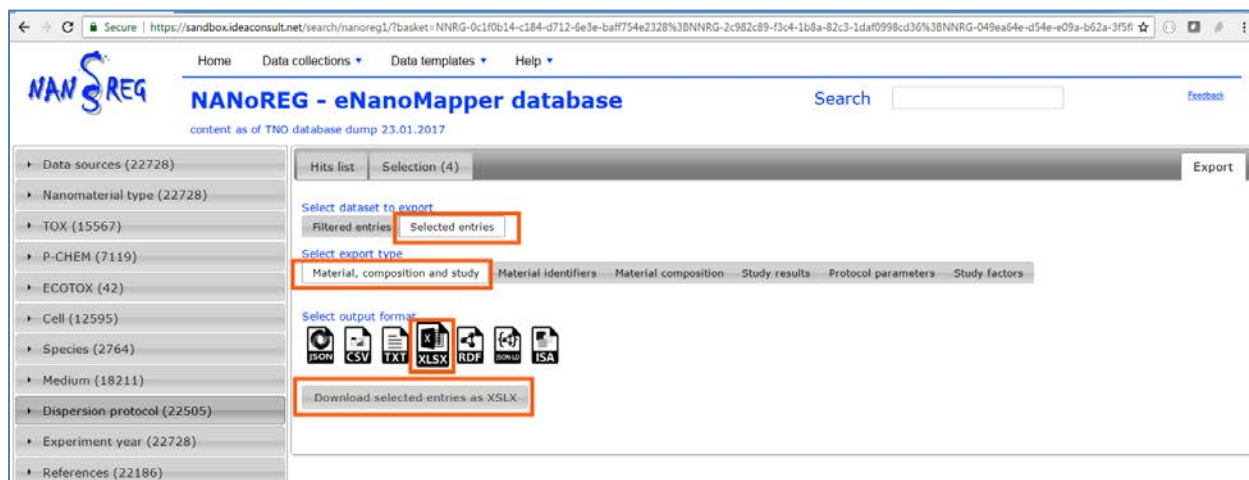


Figure 8 Export selected NM as Excel

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)

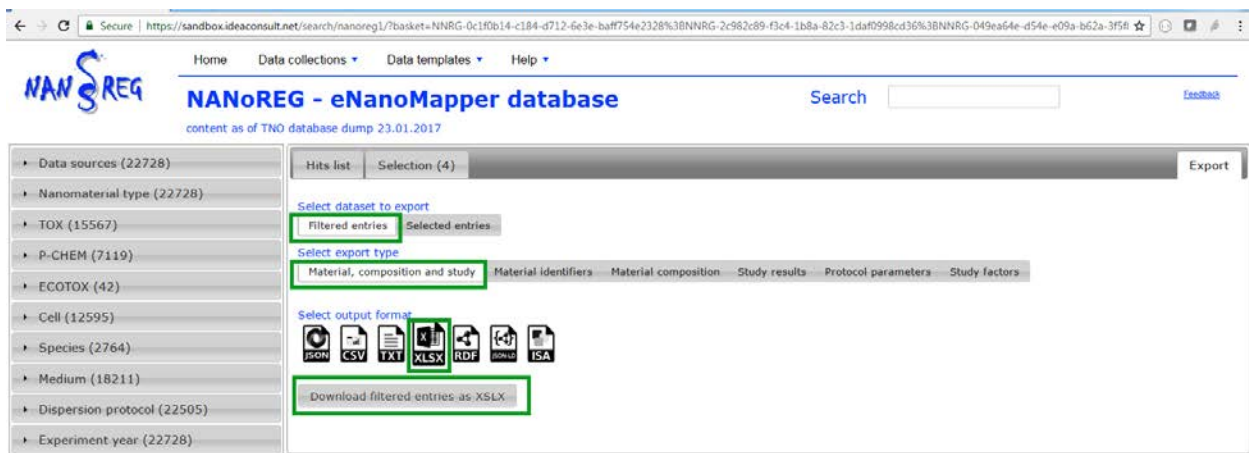


Figure 9 Export search results (filtered entries) as Excel

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, Reference, and NM type. The main content area has tabs for "Nanomaterials", "Advanced search", and "Download". A message indicates "Showing from 1 to 1 in pages of 10 substances". 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, the composition details are shown:

Composition name: TiO2 Anatase [Impurity Approx 2.3% Wt]
Composition UUID: NNRG-18280a4a-45e9-adc0-df3b-125397b1255f
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. The table has columns for Reference, Protocol, Endpoint, Result, Owner, and Reliability. Two entries are shown, both with a 'Provided' reference and 'Supplier' protocol, indicating a specific surface area of 9 m²/g. The table is part of a larger dataset showing 2 study(s) (1 to 2). The right sidebar contains links to 'Show structures', 'Remove substance', and 'Show substance', along with download options for JSON, XML, RDF, and XLSX.

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	

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

- Submit an issue to <https://github.com/enanomapper/data.enanomapper.net/labels/NANoREG%20DB>
- Or email support@ideaconsult.net

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