

eNanoMapper data management: current status

"eNanoMapper - A Database and Ontology Framework for Nanomaterials Design and Safety Assessment"

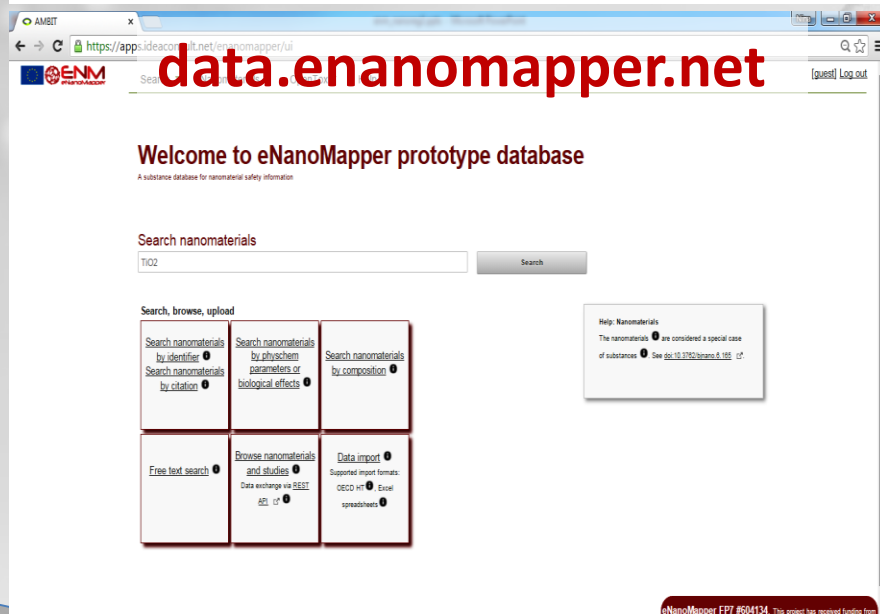
- Grant Agreement: 604134
- Duration: 36 months (1 Feb 2014 – 31 Jan 2017)

WP3. Database development and implementation

NMP.2013.1.3-2 Nanomaterials safety assessment: Ontology, database(s) for modelling and risk assessment

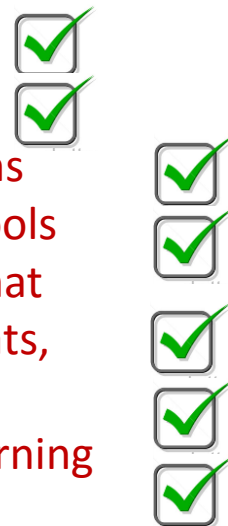
Expected impact:

(i) ... (ii) ... (iii) implementation of the database structure with all of the necessary provisions for data protection, data sharing, data quality assurance, searchability, tailored interfaces for different needs and usages, comparability and cross-talk with other databases;



eNanoMapper Vision:

- Based on OpenTox API
- Web services (multiple)
- Open Source implementations
- Bridging with data analysis tools
- Multiple data exchange format
 - ISA-TAB, semantic formats,
 - OECD HT
 - formats for machine learning packages, etc.



Databases and NM specific challenges

Database

From Wikipedia, the free encyclopedia

A **database** is an organized collection of **data**.^[1] It is the collection of schemes, **tables**, **queries**, reports, **views** and other objects. The data is typically organized to model aspects of reality in a way that supports processes requiring information, such as modelling the availability of rooms in hotels in a way that supports finding a hotel with vacancies.

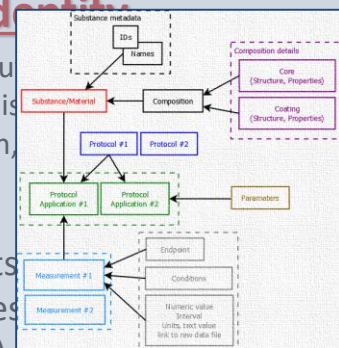
A **database management system (DBMS)** is a **computer software** application that interacts with the user, other applications, and the database itself to capture and analyze data. A general-purpose DBMS is designed to allow the definition, creation, querying, update, and

- **Physico-chemical identity**

Different analytic techniques, manufacture, mixtures, impurities, size distribution, the amount of surface modification,

- **Biological identity**

Wide variety of measurements, biological effects of ENM coronas, modes of interactions (cell lines, assays).



- **Processes requiring information**

From raw data (science) to study summaries for regulatory purposes; linking protocols to experimental protocols; risk assessment; grouping, safety-by-design

- **Different views of the data**

Requires “spreadsheet” or matrix view of data. The experimental data in the public datasets is usually not in a form appropriate for modelling (merging multiple values, conditions, similar experiments into matrix form is a challenge).

Application programming interface (API)

“substance dossier”

Data sources

1. Excel spreadsheet examples

1) Data transfer between FP7 NANoREG and eNanoMapper (WP3)

Karolinska Institutet , Prof. Bengt Fadeel lab (NANoREG WP5)

- cytotoxicity assessment of the entire panel of NANoREG nanomaterials
- All 19 nanomaterials were obtained from the JRC nanomaterial repository

2) Data transfer between FP7 MARINA and eNanoMapper (WP3)

Karolinska Institutet , Prof. Bengt Fadeel lab

- L. Farcal, F. Torres Andón, L. Di Cristo, B. M. Rotoli, O. Bussolati, E. Bergamaschi, A. Mech, N. B. Hartmann, K. Rasmussen, J. Riego-Sintes, J. Ponti, A. Kinsner-Ovaskainen, F. Rossi, A. Oomen, P. Bos, R. Chen, R. Bai, C. Chen, L. Rocks, N. Fulton, B. Ross, G. Hutchison, L. Tran, S. Mues, R. Ossig, J. Schnekenburger, L. Campagnolo, L. Vecchione, A. Pietroiusti, and B. Fadeel, "Comprehensive In Vitro Toxicity Testing of a Panel of Representative Oxide Nanomaterials: First Steps towards an Intelligent Testing Strategy," *PLoS One*, vol. 10, no. 5, p. e0127174, May 2015.

| TEST CONDITIONS | | | | | | | | | | TEST RESULTS | | | | | | | | | |
|--|--|--|--|--|--|--|--|--|--|--------------|--|--|--|--|--|--|--|--|--|
| Please complete the details below as far as possible for each set of assay results | | | | | | | | | | | | | | | | | | | |
| TEST AND END POINT - GENERAL INFO | | | | | | | | | | | | | | | | | | | |
| MARINA Work Package: VPMR | | | | | | | | | | | | | | | | | | | |
| MARINA Partner ID: P02-10 | | | | | | | | | | | | | | | | | | | |
| Test facility - Lab name etc: Division of Molecular Toxicology | | | | | | | | | | | | | | | | | | | |
| Work conducted by: email address: | | | | | | | | | | | | | | | | | | | |
| Test / Assay End-Point short description: ELISA / TNF-α release in culture medium | | | | | | | | | | | | | | | | | | | |
| End-Point Outcome metric (e.g. viability, % cell death etc): TNF-α (ng/ml) | | | | | | | | | | | | | | | | | | | |
| SOP - Protocol Name - ID (see project protocol ID list): M Documents_per_VPMRTest 9 11NANOIMMUNE_OHR_FINAL_2011 | | | | | | | | | | | | | | | | | | | |
| Test start date (dd/mm/yyyy): 11/02/12 | | | | | | | | | | | | | | | | | | | |
| Test end date (dd/mm/yyyy): 4/03/12 | | | | | | | | | | | | | | | | | | | |
| TEST SUBSTANCE | | | | | | | | | | | | | | | | | | | |
| Substance name: Titanium Dioxide TiO2 | | | | | | | | | | | | | | | | | | | |
| Standard MARINA Nanomaterial Code & Name: NM-103 (TiO2) NM-103 | | | | | | | | | | | | | | | | | | | |
| Highest concentration, in units: 100 µg/ml | | | | | | | | | | | | | | | | | | | |
| DISPERSION | | | | | | | | | | | | | | | | | | | |
| Specify the standard dispersion protocol used: NANODENOTOX Dispersion protocol (http://www.nanodenotox.eu/files/... | | | | | | | | | | | | | | | | | | | |
| Dispersion agent: water with 0.05% BSA | | | | | | | | | | | | | | | | | | | |
| Aids used to disperse - Y/N: Sonication: Y | | | | | | | | | | | | | | | | | | | |
| Treatment concentration series (C) (µg/ml): C4 10 25 | | | | | | | | | | | | | | | | | | | |
| CELL LINE/TYPE | | | | | | | | | | | | | | | | | | | |
| Short Name: HSCM (primary of human monocytes) | | | | | | | | | | | | | | | | | | | |
| Full specific name (note any line variants or related IDs): ATCC | | | | | | | | | | | | | | | | | | | |
| CELL CULTURE CONDITIONS | | | | | | | | | | | | | | | | | | | |
| Medium (Supplier/Lot No.): RPMI (Sigma, R88) | | | | | | | | | | | | | | | | | | | |
| Serum (Supplier/Lot No.): FBS (Gibco/1310) | | | | | | | | | | | | | | | | | | | |
| Serum concentration in growth medium: 10 | | | | | | | | | | | | | | | | | | | |
| Serum concentration in treatment medium: 10 | | | | | | | | | | | | | | | | | | | |
| TIME LINE | | | | | | | | | | | | | | | | | | | |
| Time points (hours - or specify any other units): T1 24 | | | | | | | | | | | | | | | | | | | |
| NOTES: including any deviations from SOP, other observations, variations etc. Add any information that will assist in the use and interpretation of the data | | | | | | | | | | | | | | | | | | | |
| Test conditions Raw data Test results Test summary | | | | | | | | | | | | | | | | | | | |



Mapping the spreadsheet content into the data model

| | A | B | C | D | E | F | G |
|----|---------------------|-------------|------------------|-----------------|-------------|----|------------------|
| 1 | TEST RESULTS | | | | | | |
| 2 | | | | | | | |
| 3 | | | | | | | |
| 4 | | Replicate 1 | | | Replicate 2 | | |
| 5 | | T1 | Titanium Dioxide | Average (ng/ml) | | T1 | Titanium Dioxide |
| 6 | | | 0 | 1.8925 | | | |
| 7 | | | 1 | 19.6985 | | | |
| 8 | | | 5 | 18.5207 | | | |
| 9 | | | 10 | 18.0280 | | | |
| 10 | | | 25 | 18.4153 | | | |
| 11 | | | 50 | 19.2965 | | | |
| 12 | | | 75 | 20.8867 | | | |
| 13 | | | 100 | 22.6964 | | | |



through JSON configuration

```
{
  "TEMPL": {
    "DATA": {
      "PARAL": {
        "SUBSTANCE_RECORD": { "...", // 7 items
        "PROTOCOL_APPLICATIONS": [
          {
            "PROTOCOL_TOP_CATEGORY": { "...", // 2 items
            "PROTOCOL_CATEGORY_CODE": { "...", // 2 items
            "PROTOCOL_GUIDELINE": { "...", // 1 item
            "PROTOCOL_ENDPOINT": { "...", // 4 items
            "RELIABILITY_STUDY_RESULT_TYPE": { "...", // 2 items
            "CITATION_TITLE": { "...", // 2 items
            "CITATION_YEAR": { "...", // 2 items
            "CITATION_OWNER": { "...", // 4 items
            "PARAMETERS": { "...", // 12 items
            "EFFECTS_BLOCK": {
              "LOCATION": {
                "ITERATION": "ABSOLUTE_LOCATION",
                "IS_ARRAY": true,
                "TRIM_ARRAY": true,
                "SHEET_INDEX": 3,
                "COLUMN_INDEX": "B",
                "ROW_INDEX": 4
              },
              "ROW_SUBBLOCKS": "= TimePoints.size()",
              "COLUMN_SUBBLOCKS": "= Replicates",
              "SUBBLOCK_SIZE_ROWS": "= C.size() + 3",
              "SUBBLOCK_SIZE_COLUMNS": 4,
              "VALUE_GROUPS": [
                {
                  "NAME": "=Assay_endpoint",
                  "UNIT": "=Outcome_metric",
                  "START_COLUMN": 3,
                  "END_COLUMN": 3,
                  "START_ROW": 3,
                  "END_ROW": "=3 - 1 + C.size()",
                  "PARAMETERS": [
                    {
                      "NAME": "Time point",
                      "ASSIGN": "ASSIGN_TO_SUBBLOCK",
                      "COLUMN_POS": 1,
                      "ROW_POS": 2,
                      "MAPPING": "Time",
                      "UNIT": "h"
                    },
                    {
                      "NAME": "Replicate",
                      "ASSIGN": "ASSIGN_TO_SU",
                      "COLUMN_POS": 1,
                      "ROW_POS": 1
                    },
                    {
                      "NAME": "Concentration",
                      "ASSIGN": "ASSIGN_TO_VALUE",
                      "COLUMN_POS": -1,
                      "ROW_POS": 0,
                      "UNIT": "µg/ml"
                    }
                  ]
                }
              ]
            }
          }
        ]
      }
    }
  }
}
```



← → C <https://apps.ideaconsult.net/enanomapper/ui/uploadsubstance1>

Search ▾ Nanomaterials ▾ OpenTox ▾ Help ▾

⌕ Substances ▸ Import ▸ Single file upload

Import new substance(s)

File (.isz or .isd or .xls or .xlsx)* No file chosen

JSON map for XLS/XLSX file No file chosen



Mapping the spreadsheet content into the data model


Discussion points

- Assay ontology annotation
- Should we include Pos/ Neg controls?
- Is this study published – what would be the correct reference?
- Is there published protocol to refer to?
- What exactly is measured?
- Cell line
- Any phys-chem data ?

through JSON configuration

```
{
  "TEMPLATE_INFO": { ... }, // 3 items
  "DATA_ACCESS": { ... }, // 9 items
  "PARALLEL_SHEETS": [ ... ], // 1 item
  "SUBSTANCE_RECORD": { ... }, // 7 items
  "PROTOCOL_APPLICATIONS": [
    {
      "PROTOCOL_TOP_CATEGORY": { ... }, // 2 items
      "PROTOCOL_CATEGORY_CODE": { ... }, // 2 items
      "PROTOCOL_GUIDELINE": { ... }, // 1 item
      "PROTOCOL_ENDPOINT": { ... }, // 4 items
      "RELIABILITY_STUDY_RESULT_TYPE": { ... }, // 2 items
      "CITATION_TITLE": { ... }, // 2 items
      "CITATION_YEAR": { ... }, // 2 items
      "CITATION_OWNER": { ... }, // 4 items
      "PARAMETERS": { ... }, // 12 items
      "EFFECTS_BLOCK": {
        "LOCATION": {
          "ITERATION": "ABSOLUTE_LOCATION",
          "IS_ARRAY": true,
          "TRIM_ARRAY": true,
          "SHEET_INDEX": 3,
          "COLUMN_INDEX": "B",
          "ROW_INDEX": 4
        },
        "ROW_SUBBLOCKS": "= TimePoints.size()",
        "COLUMN_SUBBLOCKS": "= Replicates",
        "SUBBLOCK_SIZE_ROWS": "= C.size() + 3",
        "SUBBLOCK_SIZE_COLUMNS": 4,
        "VALUE_GROUPS": [
          {
            "NAME": "=Assay_endpoint",
            "UNIT": "=Outcome_metric",
            "START_COLUMN": 3,
            "END_COLUMN": 3,
            "START_ROW": 3,
            "END_ROW": "=3 - 1 + C.size()",
            "PARAMETERS": [
              {
                "NAME": "Time point",
                "ASSIGN": "ASSIGN_TO_SUBBLOCK",
                "COLUMN_POS": 1,
                "ROW_POS": 2,
                "MAPPING": "Time",
                "UNIT": "h"
              },
              {
                "NAME": "Replicate",
                "ASSIGN": "ASSIGN_TO_SUBBLOCK",
                "COLUMN_POS": 1,
                "ROW_POS": 1
              },
              {
                "NAME": "Concentration",
                "ASSIGN": "ASSIGN_TO_VALUE",
                "COLUMN_POS": -1,
                "ROW_POS": 0,
                "UNIT": "Åµg/ml"
              }
            ]
          }
        ]
      }
    }
  ]
}
```


Data imported (MARINA/KI)


 Search ▾ Nanomaterials ▾ OpenTox ▾ Help ▾

> Search nanomaterials by identifiers

☐ Name
 ☒ Identifier
 ☐ Reference
 ☐ NM type

Nanomaterials | Advanced search | Download

Showing from 1 to 6 in pages of 10 ▾ substances
 Filter...

| | Substance Name | Substance UUID | Substance Type | Public name | Reference substance UUID | Owner | Info | | | | | | | | | | | | | | | | | | |
|---|-------------------------------|----------------------------------|----------------|-----------------------|----------------------------------|----------------------------|--|--|------|--------|---------|-----------------------|----------------------|--|----------------------|-----------|------|-----|-----------|-----------|-----------|-----------|-----------|--------------------------------------|--|
| <input type="checkbox"/> - 1 - | NM-103 (TiO2) | XLSX-7011cea0... | NPO_1486 | Titanium Dioxide | XLSX-7011cea0... | FP7 MARINA | JRC Representative Manufactured Nanomaterials = NM-103 | | | | | | | | | | | | | | | | | | |
| <input type="checkbox"/> - 2 - | NM-104 (TiO2) | XLSX-ffd24485... | NPO_1486 | Titanium Dioxide | XLSX-ffd24485... | FP7 MARINA | JRC Representative Manufactured Nanomaterials = NM-104 | | | | | | | | | | | | | | | | | | |
| <input type="checkbox"/> - 3 - | NM-110 (ZnO) | XLSX-b4e4a8e9... | NPO_1542 | Zinc Oxide | XLSX-b4e4a8e9... | FP7 MARINA | JRC Representative Manufactured Nanomaterials = NM-110 | | | | | | | | | | | | | | | | | | |
| <input type="checkbox"/> - 4 - | NM-111 (ZnO) | XLSX-fa48e134... | NPO_1542 | Zinc Oxide | XLSX-fa48e134... | FP7 MARINA | JRC Representative Manufactured Nanomaterials = NM-111 | | | | | | | | | | | | | | | | | | |
| <p> Composition name: Composition UUID: XLSX-e2468472-2757-4ad6-babb-59c82e2e8c27 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="2">Concentration ranges</th> <th>Also contained in...</th> <th>Structure</th> </tr> </thead> <tbody> <tr> <td>Core</td> <td>Zno</td> <td>215-222-5</td> <td>1314-13-2</td> <td>100 µg/ml</td> <td>0 % (w/w)</td> <td>0 % (w/w)</td> <td>Also contained in...</td> <td> $\begin{array}{c} \text{Zn} \\ \\ \text{O} \end{array}$ </td> </tr> </tbody> </table> <p style="text-align: right;">Search: <input type="text"/></p> | | | | | | | | Type | Name | EC No. | CAS No. | Typical concentration | Concentration ranges | | Also contained in... | Structure | Core | Zno | 215-222-5 | 1314-13-2 | 100 µg/ml | 0 % (w/w) | 0 % (w/w) | Also contained in... | $\begin{array}{c} \text{Zn} \\ \\ \text{O} \end{array}$ |
| Type | Name | EC No. | CAS No. | Typical concentration | Concentration ranges | | Also contained in... | Structure | | | | | | | | | | | | | | | | | |
| Core | Zno | 215-222-5 | 1314-13-2 | 100 µg/ml | 0 % (w/w) | 0 % (w/w) | Also contained in... | $\begin{array}{c} \text{Zn} \\ \\ \text{O} \end{array}$ | | | | | | | | | | | | | | | | | |
| <input type="checkbox"/> - 5 - | NM-200 (SiO2) | XLSX-93b2da85... | NPO_1373 | Silica Dioxide | XLSX-93b2da85... | FP7 MARINA | JRC Representative Manufactured Nanomaterials = NM-200 | | | | | | | | | | | | | | | | | | |
| <input type="checkbox"/> - 6 - | NM-203 (SiO2) | XLSX-aacd8ad8... | NPO_1373 | Silica Dioxide | XLSX-aacd8ad8... | FP7 MARINA | JRC Representative Manufactured Nanomaterials = NM-203 | | | | | | | | | | | | | | | | | | |



From spreadsheets to DB content

FP7 MARINA /KI

doi:10.1371/journal.pone.0127174

Farcal et al. 2015

TEST CONDITIONS
In-Vitro Template

Please complete the details below as far as possible for each set of assay results

While we need to standardise MARINA toxicology data records as far as possible for compatibility, some You can add additional items below where necessary for further replicates, concentrations, timepoints or in the notes area or adjacent to data tables, add annotations where it would be helpful to flag significant

TEST AND END POINT - GENERAL INFO

MARINA Work Package: WP09
MARINA Partner ID: P32-KI
Test facility - Lab name etc: Division of Molecular Toxicology
Work conducted by: email address

End-Point short description: ELISA / TNF- α release in culture medium
TNF- α assay description form

% viability, % cell death etc: P is derived
TNF- α (ng/ml)

see project protocol ID list: M:Documents_per WP09/P32-KI 9 11/2012
1st start date (dd/mm/yyyy): 4/30/2013
1st end date (dd/mm/yyyy):

TEST SUBSTANCE

Substance name: Titanium Dioxide TiO₂
CAS No: 1344-76-2
Standard MARINA Nanomaterial Code & Name: NM-103 (TiO₂) NM-103
(See MARINA Materials list)

Highest concentration, in units: 100 μ g/ml

DISPERSION

Specify the standard dispersion protocol used: (or otherwise specify the dispersion technique used)
NANOGENOTOX Dispersion protocol (http://www.nanogenotox.eu/)

Dispersion agent: water with 0.05% BSA

Aids used to disperse - Y/N: Sonication: N Vortexing: Y

Treatment concentration series (C) (g/ml): C1: 0 C2: 1 C3: 5 C4: 10 C5: 25 C6: 50 C7: 75 C8: 100

CELL LINE/TYPE

Short-name: HMDM (primary cells)
Full specific name (note any line variants or related IDs): human monocyte-derived macrophages (HMDM) ATCC

CELL CULTURE CONDITIONS

Medium (Supplier/Lot No.): RPMI (Sigma) 882729
Serum (Supplier/Lot No.): FBS (Gibco) 15105K
Serum concentration in growth medium: 10%
Serum concentration in treatment medium:

TIMELINE

Time points (hours - or specify any other units): T1
Alter or add as necessary: 24

NOTES - including any deviations from SOPs, other observations, variations etc. Add any information that

Test conditions Raw data Test results Test summary

TEST RESULTS

| Replicate | Titanium Dioxide | Average (ng/ml) | Replicate | Titanium Dioxide | Average (ng/ml) | Replicate | Titanium Dioxide | Average (ng/ml) | Replicate | Titanium Dioxide | Average (ng/ml) |
|-----------|------------------|-----------------|-----------|------------------|-----------------|-----------|------------------|-----------------|-----------|------------------|-----------------|
| T1 | 0 | 1.8925 | T1 | 0 | -0.3425 | T1 | 0 | 2.189 | T1 | 0 | 9.502 |
| | 1 | 19.6985 | | 1 | 5.9887 | | 1 | 2.474 | | 1 | 8.808 |
| | 5 | 18.5207 | | 5 | 5.7696 | | 5 | 2.002 | | 5 | 8.957 |
| | 10 | 18.0280 | | 10 | 5.3011 | | 10 | 1.786 | | 10 | 8.306 |
| | 25 | 18.4153 | | 25 | 5.1602 | | 25 | 1.570 | | 25 | 8.244 |
| | 50 | 19.2965 | | 50 | 5.2292 | | 50 | 1.735 | | 50 | 9.507 |
| | 75 | 20.8867 | | 75 | 6.1564 | | 75 | 1.290 | | 75 | 14.416 |
| | 100 | 22.6964 | | 100 | 7.2811 | | 100 | 1.206 | | 100 | 15.438 |

IUC Substance: Composition: Tox (2)

Filter...

Titanium Dioxide

NPO_1709 LDH Release Assay (1)

BAO_0002993 Cytotoxicity Assay (1)

| Reference | Protocol | Endpoint | Result | Concentration | Time point | Replicate | Owner |
|-----------|----------|---|--------------|----------------|------------|-------------|-------|
| | | TNF- α (ng/ml) | 1.893 ng/ml | 0 μ g/ml | 24 h | Replicate 1 | |
| | | TNF- α (ng/ml) | 19.698 ng/ml | 1 μ g/ml | 24 h | Replicate 1 | |
| | | TNF- α (ng/ml) | 18.521 ng/ml | 5 μ g/ml | 24 h | Replicate 1 | |
| | | TNF- α (ng/ml) | 18.028 ng/ml | 10 μ g/ml | 24 h | Replicate 1 | |
| | | TNF- α (ng/ml) | 18.415 ng/ml | 25 μ g/ml | 24 h | Replicate 1 | |
| | | Aids used to disperse/stirring: Y | 19.297 ng/ml | 50 μ g/ml | 24 h | Replicate 1 | |
| | | Cell line: HMDM (primary cells) | 20.887 ng/ml | 75 μ g/ml | 24 h | Replicate 1 | |
| | | Cell line/type - supplier: ATCC | 22.696 ng/ml | 100 μ g/ml | 24 h | Replicate 1 | |
| | | Cell culture conditions - Serum | -0.343 ng/ml | 0 μ g/ml | 24 h | Replicate 2 | |
| | | FBS (Gibco/413105K) | 5.989 ng/ml | 1 μ g/ml | 24 h | Replicate 2 | |
| | | Cell culture conditions - Serum | 5.77 ng/ml | 5 μ g/ml | 24 h | Replicate 2 | |
| | | concentration in treatment | 5.301 ng/ml | 10 μ g/ml | 24 h | Replicate 2 | |
| | | medium: 0.1 | 5.16 ng/ml | 25 μ g/ml | 24 h | Replicate 2 | |
| | | Cell culture conditions - Serum | 5.229 ng/ml | 50 μ g/ml | 24 h | Replicate 2 | |
| | | concentration in growth medium: 0.1 | 6.156 ng/ml | 75 μ g/ml | 24 h | Replicate 2 | |
| | | Cell line/Type - Full name: human monocyte-derived macrophages (HMDM) | 7.281 ng/ml | 100 μ g/ml | 24 h | Replicate 2 | |
| | | Dispersion agent: water with 0.05% BSA | 2.189 ng/ml | 0 μ g/ml | 24 h | Replicate 3 | |
| | | Aids used to disperse/vortexing: N | 2.474 ng/ml | 1 μ g/ml | 24 h | Replicate 3 | |
| | | | 2.002 ng/ml | 5 μ g/ml | 24 h | Replicate 3 | |
| | | Aids used to disperse/sonication: N | 1.786 ng/ml | 10 μ g/ml | 24 h | Replicate 3 | |
| | | Dispersion protocol: NANOGENOTOX Dispersion protocol | 1.57 ng/ml | 25 μ g/ml | 24 h | Replicate 3 | |
| | | (http://www.nanogenotox.eu/files/PDF/web%20nanogenotox%20dispersion%20protocol.pdf) | 1.735 ng/ml | 50 μ g/ml | 24 h | Replicate 3 | |
| | | Cell culture conditions - medium: RPMI (Sigma, N8882729) | 1.29 ng/ml | 75 μ g/ml | 24 h | Replicate 3 | |
| | | | 1.206 ng/ml | 100 μ g/ml | 24 h | Replicate 3 | |
| | | | 9.502 ng/ml | 0 μ g/ml | 24 h | Replicate 4 | |
| | | | 8.808 ng/ml | 1 μ g/ml | 24 h | Replicate 4 | |
| | | | 8.957 ng/ml | 5 μ g/ml | 24 h | Replicate 4 | |
| | | | 8.306 ng/ml | 10 μ g/ml | 24 h | Replicate 4 | |
| | | | 8.244 ng/ml | 25 μ g/ml | 24 h | Replicate 4 | |
| | | | 9.507 ng/ml | 50 μ g/ml | 24 h | Replicate 4 | |

Additional File 1_Table S1.docx

- MARINA-invito-WP09-P32-NM103TiO2-HMDM_Cytokines_TNF α .xls
- MARINA-invito-WP09-P32-NM103TiO2-HMDM_Cytotoxicity_LDH.xls
- MARINA-invito-WP09-P32-NM104TiO2-HMDM_Cytokines_TNF α .xls
- MARINA-invito-WP09-P32-NM104TiO2-HMDM_Cytotoxicity_LDH.xls
- MARINA-invito-WP09-P32-NM110ZnO-HMDM_Cytokines_TNF α .xls
- MARINA-invito-WP09-P32-NM110ZnO-HMDM_Cytotoxicity_LDH.xls
- MARINA-invito-WP09-P32-NM111ZnO-HMDM_Cytokines_TNF α .xls
- MARINA-invito-WP09-P32-NM111ZnO-HMDM_Cytotoxicity_LDH.xls
- MARINA-invito-WP09-P32-NM200SiO2-HMDM_Cytokines_TNF α .xls
- MARINA-invito-WP09-P32-NM200SiO2-HMDM_Cytotoxicity_LDH.xls
- MARINA-invito-WP09-P32-NM203SiO2-HMDM_Cytokines_TNF α .xls
- MARINA-invito-WP09-P32-NM203SiO2-HMDM_Cytotoxicity_LDH.xls
- TableS1.xlsx

ENM

Search * Nanomaterials * OpenTox * Help *

Search nanomaterials by Identifiers

Advanced search Download

Showing from 1 to 6 in pages of 10 substances Previous Next

| Substance | Substance Name | Substance Type | Public name | Reference substance UUID | Owner | Info |
|-----------|----------------------------|------------------|-------------|--------------------------|------------------|---|
| 1 - | NM-103 (TiO ₂) | XLX-7011ce9-... | NPO_1486 | Titanium Dioxide | XLX-7011ce9-... | EP2 MARINA JRC Representative Manufactured Nanomaterials = NM-103 |
| 2 - | NM-104 (TiO ₂) | XLX-f424485-... | NPO_1486 | Titanium Dioxide | XLX-f424485-... | EP2 MARINA JRC Representative Manufactured Nanomaterials = NM-104 |
| 3 - | NM-110 (ZnO) | XLX-lb4e8a9-... | NPO_1542 | Zinc Oxide | XLX-lb4e8a9-... | EP2 MARINA JRC Representative Manufactured Nanomaterials = NM-110 |
| 4 - | NM-111 (ZnO) | XLX-fa58e13d-... | NPO_1542 | Zinc Oxide | XLX-fa58e13d-... | EP2 MARINA JRC Representative Manufactured Nanomaterials = NM-111 |
| 5 - | NM-200 (SiO ₂) | XLX-93b2da85-... | NPO_1373 | Silica Dioxide | XLX-93b2da85-... | EP2 MARINA JRC Representative Manufactured Nanomaterials = NM-200 |
| 6 - | NM-203 (SiO ₂) | XLX-aacdfad8-... | NPO_1373 | Silica Dioxide | XLX-aacdfad8-... | EP2 MARINA JRC Representative Manufactured Nanomaterials = NM-203 |

Composition name: Composition UUID: XLX-c2468472-2757-4a6b-babb-59c82e2e8c27

Purity of IUC Substance:

| Type | Name | EC No. | CAS No. | Typical concentration | Concentration ranges | Structure |
|------|------|-----------|-----------|-----------------------|----------------------|-------------------|
| Cure | Zn | 215-232-9 | 1314-13-2 | 100 μ g/ml | 0 % (w/v) 0 % (w/v) | <chem>[Zn]</chem> |

Search:



Data sources 2. PDF files



| Summary of physico-chemical data | | | |
|---|---|---|----------|
| Physico-chemical property (if applicable) | Description of physico-chemical properties (if applicable) | Source of information | Date |
| Shape | TEM: Primary subunits tend to be more or less equi-axed. The 3D structure suggests they are spherical or ellipsoidal [2] Aggregates/agglomerates have a more fractal-like structure [1-2] and minor amounts of singlet spheroidal particles [1] | [1] NANOGENOTOX: NRCWE data [2] JRC technical report | 28.01.14 |
| Core size distribution | TEM: 110 ± 57 nm [1]- from 20 to | [1] NANOGENOTOX- | 28.01.14 |

Phys-chem characterisation of representative materials
JRC Nanomaterials Repository
Juan Riego-Sintes
<https://ec.europa.eu/jrc/en/scientific-tool/jrc-nanomaterials-repository>

BET: 10.03 m²/g (room temp) [2]
Deliverable 4.4
[2] JRC technical report

| A | B | C | D | E | F | G | H |
|---|--------------|-------------------------|--|-------|------------------------|------------------------------|---|
| Physico-chemical property | Protocol | Endpoint | Description of physico-chemical properties | Units | Experimental condition | Experimental condition value | |
| 1 Shape | TEM | Shape | Primary subunits tend to be more or less equi-axed. The 3D structure suggests they are spherical or ellipsoidal | | | | |
| 2 Shape | TEM | Shape | Aggregates/agglomerates have a more fractal-like structure [1-2] and minor amounts of singlet spheroidal particles | | | | |
| 3 Shape | TEM | Shape | 10 ± 57 | | | | |
| 4 Core size distribution | TEM | Size | | | | | |
| 5 Core size distribution | TEM | Size | 20 | | | | |
| 6 Core size distribution | XRD | Size | 56 | | | | |
| 7 Core size distribution | TEM | Size | ~300 nm | | | | |
| 8 Core size distribution | TEM | Size | <50 nm | | | | |
| 9 Core size distribution | TEM | Size | <30 nm | | | | |
| 10 Core size distribution | TEM | Aggregates/agglomerates | 30 | | | | |
| 11 Aspect ratio | TEM | Aspect ratio | 1.35 | | | | |
| 12 Surface morphology/topography | | | | | | | |
| 13 Specific surface area | BET | Specific surface area | | | | | |
| 14 Specific surface area | BET | Specific surface area | 10.0 | | | | |
| 15 Crystallite structure | XRD | | | | | | |
| 16 Core material (elemental composition) | EDS | Ti | | | | | |
| 17 Core material (elemental composition) | EDS | O | | | | | |
| 18 Overall material composition (including degree of purity, ICP-OES) | EDS | Fe | | | | | |
| 19 Overall material composition (including degree of purity, ICP-OES) | EDS | Si | | | | | |
| 20 Overall material composition (including degree of purity, ICP-OES) | EDS | P | | | | | |
| 21 Overall material composition (including degree of purity, ICP-OES) | EDS | K | | | | | |
| 22 Overall material composition (including degree of purity, ICP-OES) | EDS | Al | | | | | |
| 23 Overall material composition (including degree of purity, ICP-OES) | EDS | Cr | | | | | |
| 24 Overall material composition (including degree of purity, ICP-OES) | EDS | K | | | | | |
| 25 Overall material composition (including degree of purity, ICP-OES) | EDS | P | | | | | |
| 26 Overall material composition (including degree of purity, ICP-OES) | EDS | Zr | | | | | |
| 27 Overall material composition (including degree of purity, ICP-OES) | EDS | Ca | | | | | |
| 28 Overall material composition (including degree of purity, ICP-OES) | EDS | Na | | | | | |
| 29 Coating | TGA | | | | | | |
| 30 Functional groups present on the coating | | | | | | | |
| 31 Zeta potential | DLS | ZETA POTENTIAL | -49 | | | | |
| 32 Hydrodynamic radius | DLS | HYDRODYNAMIC RADH | 215 | | | | |
| 33 Hydrodynamic radius | DLS | HYDRODYNAMIC RADH | 210 | | | | |
| 34 Surface area | BET | Nitrogen BET adsorption | | | | | |
| 35 Heavy metals contaminants | ICP analysis | P | | | | | |

```

{
  "TEMPLATE_INFO": { ... }, // 3 items
  "DATA_ACCESS": {
    "ITERATION": "ROW_SINGLE",
    "SHEET_INDEX": 1,
    "START_ROW": 5,
    "END_ROW": 10,
    "START_HEADER_ROW": 2,
    "END_HEADER_ROW": 3,
    "ALLOW_EMPTY": true,
    "RECOGNITION": "BY_INDEX"
  },
  "SUBSTANCE_RECORD": { ... }, // 5 items
  "PROTOCOL_APPLICATIONS": [
    {
      "CITATION_TITLE": {
        "COLUMN_INDEX": "Q"
      },
      "PROTOCOL_GUIDELINE": {
        "guideline1": {
          "COLUMN_INDEX": "Q"
        }
      },
      "PROTOCOL_ENDPOINT": {
        "COLUMN_INDEX": "P"
      },
      "PARAMETERS": {
        "Dispersion": {
          "COLUMN_INDEX": "J"
        },
        "Sample Provider": {
          "COLUMN_INDEX": "O"
        }
      },
      "EFFECTS": [ ... ] //
    }
  ]
}

```

| Reference | Protocol | Endpoint | Result | Owner |
|-----------|----------|---------------|-------------|----------|
| DOI | | PARTICLE SIZE | (42, 90) nm | NanoWiki |
| DOI | | PARTICLE SIZE | 267 nm | NanoWiki |

https://apps.ideaconsult.net/enanmapper/ui/uploadsubstance1

Substances Import Single file upload

Import new substance(s)

File (.isz or .isd or .xls or .xlsx)

JSON map for XLS/XLSX file

Choose File No file chosen

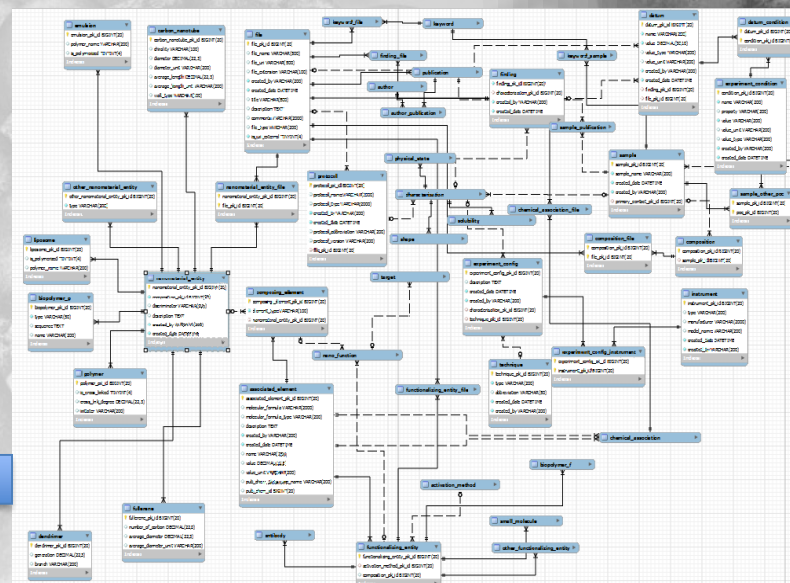
Choose File No file chosen

Submit



Data sources 3. SQL database (e.g. caNanoLab)

- MySQL dump provided to eNanoMapper
- Domain model class names and attributes
<https://cdebrowser.nci.nih.gov/CDEBrowser/>
- Definitions for caNanoLab concepts are maintained in the NCI Enterprise Vocabulary Services
<https://ncit.nci.nih.gov/ncitbrowser>
- Code: <https://github.com/NCIP/cananolab>



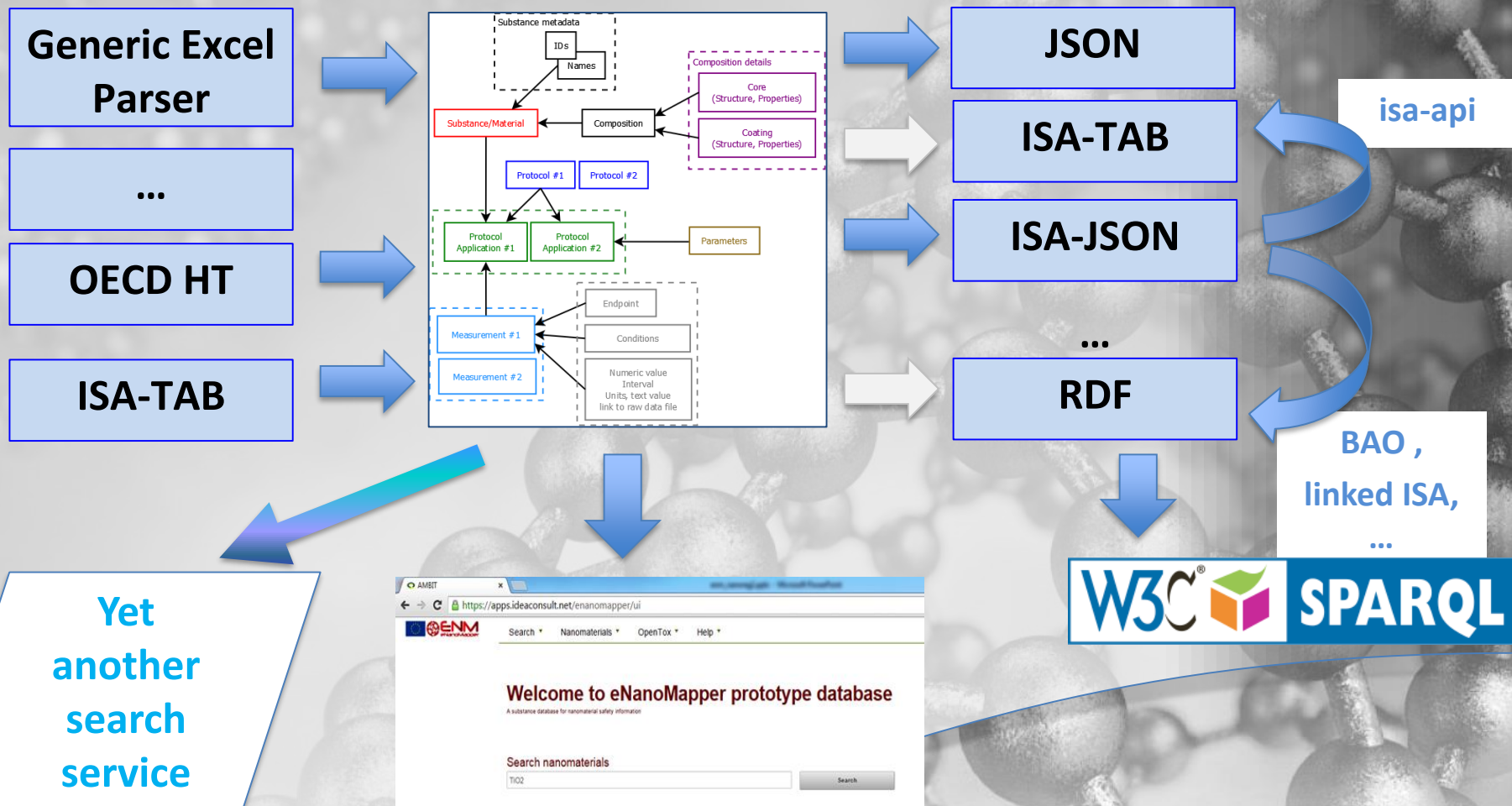
Mapping into eNanoMapper data model

The screenshot shows the eNanoMapper web interface. On the left, there is a sidebar with a search bar and a list of filters. The main area displays a table of search results. The table has columns for Substance Name, Substance UUID, Substance Type, Public name, Owner, and Info. The results are sorted by Substance Name.

| | Substance Name | Substance UUID | Substance Type | Public name | Owner | Info |
|----|-------------------------------------|------------------|----------------|-------------------------------------|----------|------|
| 1 | MIT_HGH-JMcCarthyHL2005-01 | CNHL-fa79e308... | - | MIT_HGH-JMcCarthyHL2005-01 | 15695883 | |
| 2 | MIT_HGH-JMcCarthyHL2005-02 | CNHL-818a4c8c... | - | MIT_HGH-JMcCarthyHL2005-02 | 15695883 | |
| 3 | GT_EM-HDuanJACS2007-01 | CNHL-bdbd73cf... | - | GT_EM-HDuanJACS2007-01 | 15695922 | |
| 4 | GT_EM-HDuanJACS2007-02 | CNHL-91563398... | - | GT_EM-HDuanJACS2007-02 | 15695922 | |
| 5 | GT_EM-HDuanJACS2007-03 | CNHL-09919cc2... | - | GT_EM-HDuanJACS2007-03 | 15695922 | |
| 6 | NEU-LWangJMBT2008-02 | CNHL-681de79f... | - | NEU-LWangJMBT2008-02 | 15695958 | |
| 7 | UAM-CSIC_IMDEA-AVillanuevaHT2009-01 | CNHL-88579c37... | - | UAM-CSIC_IMDEA-AVillanuevaHT2009-01 | 15695943 | |
| 8 | UAM-CSIC_IMDEA-AVillanuevaHT2009-03 | CNHL-886f923c... | - | UAM-CSIC_IMDEA-AVillanuevaHT2009-03 | 15695943 | |
| 9 | NIOSH-VWalkerTAP2009-02 | CNHL-00704f6c... | - | NIOSH-VWalkerTAP2009-02 | 15695979 | |
| 10 | KI-HKarlssonCRT2008-01 | CNHL-84e50771... | - | KI-HKarlssonCRT2008-01 | 14811136 | |
| 11 | KI-HKarlssonCRT2008-03 | CNHL-1d676b8b... | - | KI-HKarlssonCRT2008-03 | 14811136 | |
| 12 | KI-HKarlssonCRT2008-05 | CNHL-59a8b8b0... | - | KI-HKarlssonCRT2008-05 | 14811136 | |



eNanoMapper data format conversion



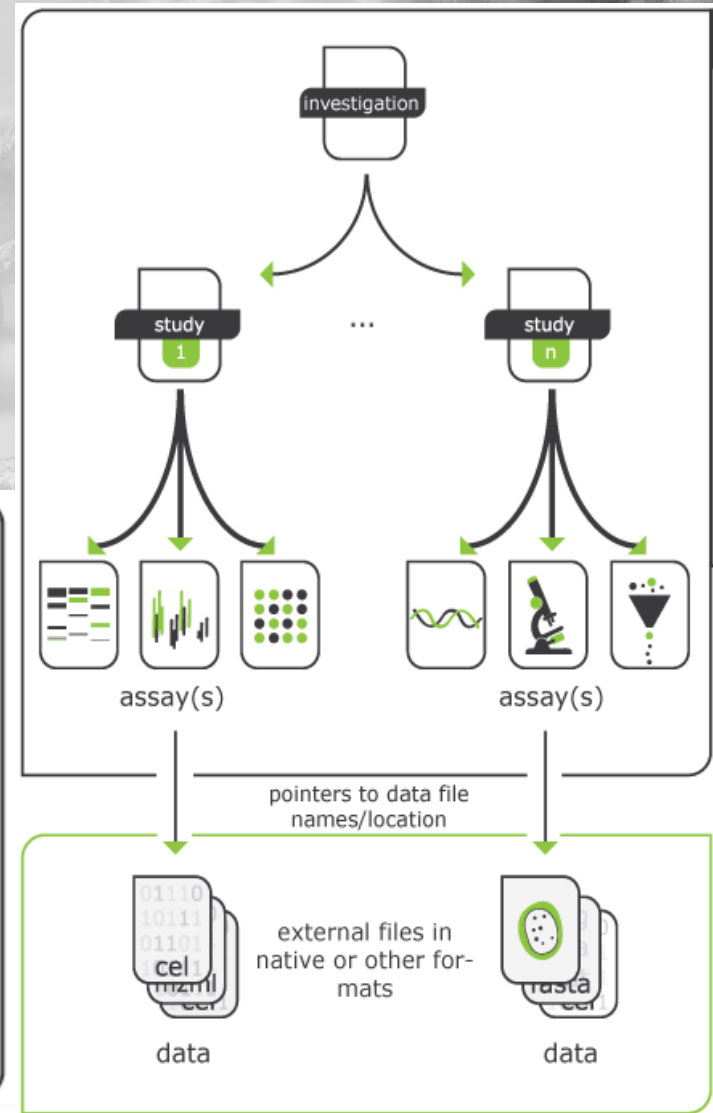
ISA-TAB: Susanna-Assunta Sansone et. al., **Toward interoperable bioscience data**, Nature Genetics 44, 121–126 (2012)

- Version 1 (Nov 2008)
- Data is described in 3 layers
- Tab delimited format (*.txt and *.xls/xlsx)
- Only meta data is stored
- Pointers to the data files
- Ontology references
- Additional configurations
- Version 2 (2015)
- (under development)
- ISA-JSON (2015)
- (under development)

investigation
high level concept to link related studies

study
the central unit, containing information on the subject under study, its characteristics and any treatments applied.
a study has associated assays

assay
test performed either on material taken from the subject or on the whole initial subject, which produce qualitative or quantitative measurements (data)





(Investigation file)

| | A | B |
|----|--|---|
| 1 | ONTOLOGY SOURCE REFERENCE | |
| 2 | Term Source Name | CHEBI |
| 3 | Term Source File | http://data.bioontology.org/ontologies/CHEBI |
| 4 | Term Source Version | 78 |
| 5 | Term Source Description | Chemical Entities of Biological Interest Ontology |
| 6 | INVESTIGATION | |
| 7 | Investigation Identifier | BII-I-1 |
| 8 | Investigation Title | Growth control of the eukaryote cell: a systems biology study in yeast |
| 9 | Investigation Description | Background Cell growth underlies many key cellular and development |
| 10 | Investigation Submission Date | 4/30/2007 |
| 11 | Investigation Public Release Date | 3/10/2009 |
| 12 | Comment [Created with configuration] | |
| 13 | Comment [Last Opened With Configuration] | isaconfig-default_v2013-02-13 |
| 14 | Comment [Owning Organisation URI] | |
| 15 | Comment [Consortium URI] | |
| 16 | Comment [Principal Investigator URI] | |
| 17 | Comment [Investigation keywords] | |
| 18 | INVESTIGATION PUBLICATIONS | |
| 19 | Investigation PubMed ID | 17439666 |
| 20 | Investigation Publication DOI | doi:10.1186/jbiol54 |
| 21 | Investigation Publication Author List | Castrillo JI, Zeef LA, Hoyle DC, Zhang N, Hayes A, Gardner DC, Cornell M |
| 22 | Investigation Publication Title | Growth control of the eukaryote cell: a systems biology study in yeast |
| 23 | Investigation Publication Status | indexed in Pubmed |
| 24 | Investigation Publication Status Term Accession Number | |



(study and assay files)

Investigation consists of one or more studies

| | |
|---|---|
| Study Person Roles Term Source REF | |
| Comment[Study Person REF] | |
| STUDY | |
| Study Identifier | BII-S-2 |
| Study Title | A time course analysis of transcription response in yeast treated with r |
| Study Description | Comprehensive high-throughput analyses at the levels of mRNAs, prot |
| Comment[Study Grant Number] | |
| Comment[Study Funding Agency] | |
| Study Submission Date | 4/30/2007 |
| Study Public Release Date | 3/10/2009 |
| Study File Name | s_BII-S-2.txt |
| STUDY DESIGN DESCRIPTORS | |
| Study Design Type | time series design |
| Study Design Type Term Accession Number | http://purl.obolibrary.org/obo/OBI_0500020 |
| Study Design Type Term Source REF | OBI |
| STUDY PUBLICATIONS | |

pointer to the study file

Each study contains one or more assays

| | | | |
|--|---|---|-------------------------|
| STUDY ASSAYS | | | |
| Study Assay File Name | a_metabolome.txt | a_proteome.txt | a_transcriptome.txt |
| Study Assay Measurement Type | metabolite profiling | protein expression profiling | transcription profiling |
| Study Assay Measurement Type Term Accession Number | http://purl.obolibrary.org/obo/OBI_00 | http://purl.obolibrary.org/o | 42 |

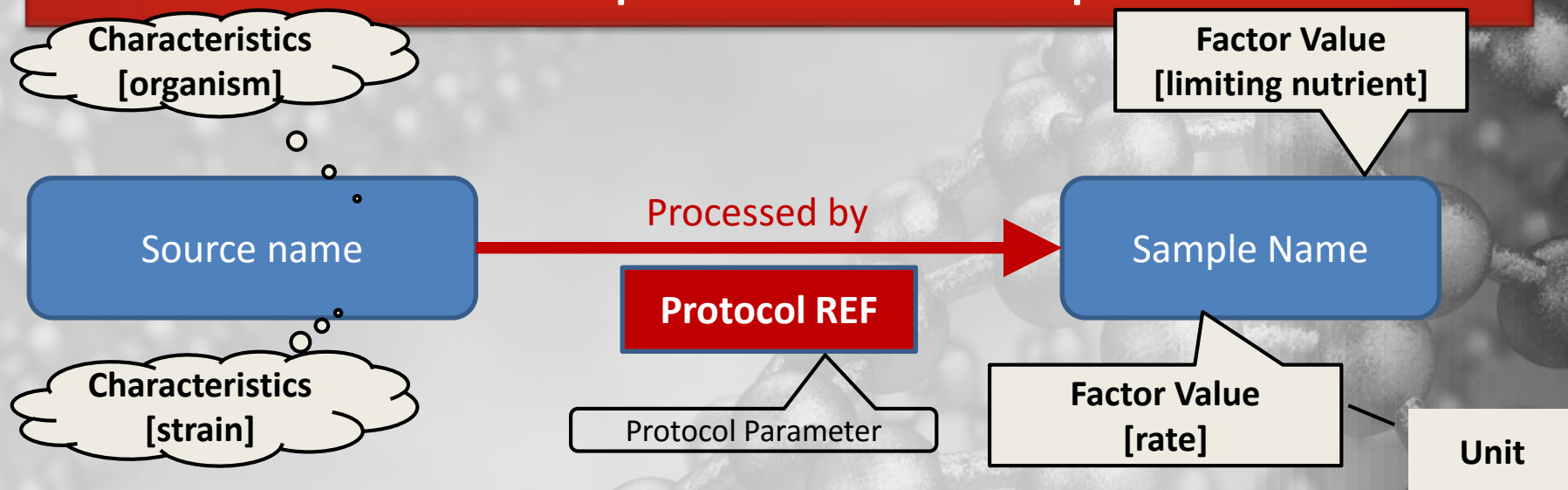
pointers to the assay files





data model:

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

The ISA-TAB-Nano project is an effort of the
National Cancer Institute (**NCI**) National Cancer
Informatics Program (**NCIP**) Nanotechnology
Informatics Working Group (**Nano WG**)



- **ISA-TAB-Nano site**

<https://wiki.nci.nih.gov/display/ICR/ISA-TAB-Nano>

- ISA-TAB-Nano templates to create ISA-TAB-Nano files
- Template glossary for definitions
- Example files

- Publications

- BMC Biotechnology 2013, 13:2
<http://www.biomedcentral.com/1472-6750/13/2/abstract>
- Commentary Nature Nanotechnology 2013, 8, 73-74
<http://www.nature.com/nnano/journal/v8/n2/full/nnano.2013.12.htm>

[illegible]

ISA-TAB-Nano



Material M is comprised of A, B, and C

| Material Source Name | Material Name | Material Constituent | Material Linkage Type |
|----------------------|---------------|----------------------|-----------------------|
| M-lab-1 | M | A;B;C | |
| M-lab-1 | M | A;B | covalent linkage |
| M-lab-1 | M | A; C | covalent linkage |
| M-lab-1 | A | | |
| M-lab-1 | B | | |
| M-lab-1 | C | | |

Material M is comprised of A, B, and C within Material M, A and B are linked and A and C are linked

ISA-JSON project



<https://github.com/ISA-tools/isa-api>

- Under development by Oxford group and collaborators
 - Python based **ISA** API library
 - New data format based on JSON describes the ISA experimental graph
 - More efficient data storage than the TAB delimited
 - Full support of the old ISA-TAB format (v.1)
 - New extended ISA v.2
- eNM – ISA-Tab team meeting May 2015 (EBI)
 - ISA-Tab hackathon July 2015
 - eNM- ISA-Tab team virtual meeting Nov 3 2015
 - ISA Working group teleconference Dec 9 2015
 - Active collaboration on github
 - schema, issues, code



ISA-JSON schemas



https://github.com/ISA-tools/isa-api/tree/master/isatools/schemas/isa_model_version_1_0_schemas/core

assay_schema.json

comment_schema.json

data_schema.json

factor_schema.json

factor_value_schema.json

investigation_schema.json

material_attribute_schema.json

material_schema.json

ontology_annotation_schema.json

ontology_source_reference_schema.json

organization_schema.json

parameter_schema.json

person_schema.json

process_schema.json

protocol_schema.json

```
{
  "$schema": "http://json-schema.org/draft-04/schema",
  "title": "ISA investigation schema",
  "description": "JSON-schema representing an investigation in the ISA model",
  "type": "object",
  "properties": {
    "identifier": { "type": "string" },
    "title": { "type": "string" },
    "description": { "type": "string" },
    "submissionDate": { "type": "string", "format": "date-time" },
    "publicReleaseDate": { "type": "string", "format": "date-time" },
    "commentCreatedWithConfiguration": {
      "$ref": "comment_schema.json#",
      "name": "Created With Configuration"
    },
    "commentLastOpenedWithConfiguration": {
      "$ref": "comment_schema.json#",
      "name": "Last Opened With Configuration"
    },
    "ontologySourceReferences": {
      "type": "array",
      "items": {
        "$ref": "ontology_source_reference_schema.json#"
      }
    }
  }
}
```


eNanoMapper: ISA-JSON material extension

The screenshot shows the GitHub repository page for `enanmapper/isa-api`, which is forked from `ISA-tools/isa-api`. The repository has 18 pull requests, 0 stars, and 2 forks. The current branch is `master`. The commit history shows the following changes:

| Commit | Message | Time |
|-------------------------------------|--|-------------|
| ntk73 added constituent_schema.json | added constituent_schema.json | a month ago |
| .. | .. | .. |
| material_schema.json | Added basic properties of material json-schema | a month ago |

A blue arrow points from the commit history to a callout box on the right.

Contributing new
extension to isa-api
(under development
by eNM team)

JSON schema corresponding
to ISA-TAB-Nano
material file



eNanoMapper: ISA (v.1) Java classes

- Assay.java
- Comment.java
- Component.java
- Data.java
- Factor.java
- FactorValue.java
- Investigation.java
- Material.java
- MaterialAttribute.java
- MeasurementType.java
- OntologyAnnotation.java
- OntologySourceReference.java
- Organization.java
- Parameter.java
- Person.java
- Process.java
- Protocol.java
- Publication.java
- Role.java
- Sample.java
- Source.java
- Study.java
- TechnologyType.java
- Value.java

Investigation.java

- Investigation
 - commentCreatedWithConfiguration
 - commentLastOpenedWithConfiguration
 - description
 - identifier
 - ontologySourceReferences
 - people
 - publications
 - publicReleaseDate
 - studies
 - submissionDate
 - title

```
@JsonProperty("identifier")
public String identifier;
@JsonProperty("title")
public String title;
@JsonProperty("description")
public String description;
@JsonProperty("submissionDate")
public Date submissionDate;
@JsonProperty("publicReleaseDate")
public Date publicReleaseDate;

@JsonProperty("commentCreatedWithConfiguration")
public Comment commentCreatedWithConfiguration;
@JsonProperty("commentLastOpenedWithConfiguration")
public Comment commentLastOpenedWithConfiguration;
@JsonProperty("ontologySourceReferences")
public List<OntologySourceReference> ontologySourceReferences = new ArrayList<>();
@JsonProperty("publications")
public List<Publication> publications = new ArrayList<Publication>();
@JsonProperty("people")
public List<Person> people = new ArrayList<Person>();
@JsonProperty("studies")
public List<Study> studies = new ArrayList<Study>();
}
```

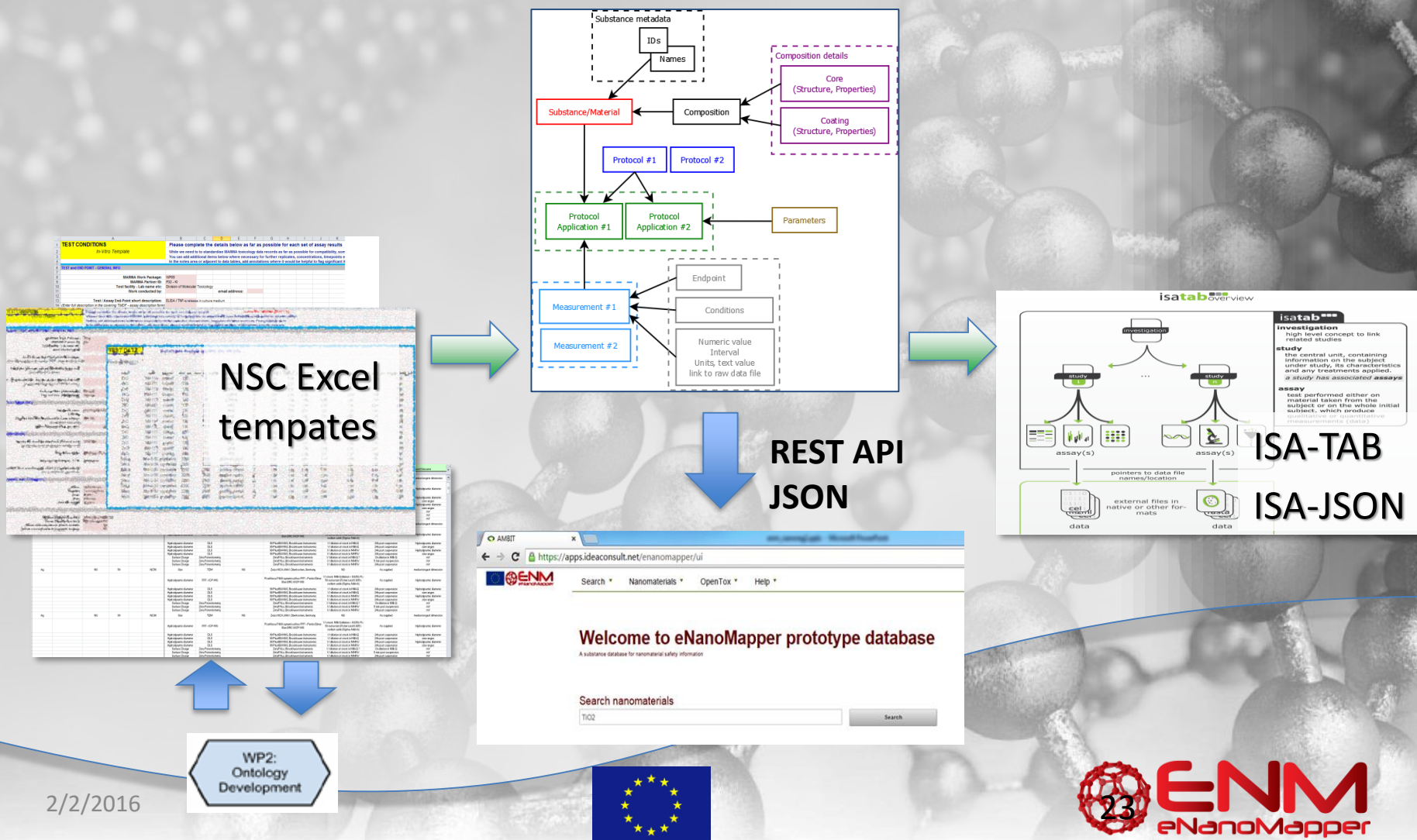
Study.java

- Study
 - assays
 - description
 - identifier
 - people
 - processSequence
 - protocols
 - publications
 - publicReleaseDate
 - samples
 - sources
 - studyDesignDescriptors
 - submissionDate
 - title

```
public class Study {

    @JsonProperty("identifier")
    public String identifier;
    @JsonProperty("title")
    public String title;
    @JsonProperty("description")
    public String description;
    @JsonProperty("submissionDate")
    public Date submissionDate;
    @JsonProperty("publicReleaseDate")
    public Date publicReleaseDate;
    @JsonProperty("publications")
    public List<Publication> publications = new ArrayList<Publication>();
    @JsonProperty("people")
    public List<Person> people = new ArrayList<Person>();
    @JsonProperty("studyDesignDescriptors")
    public List<OntologyAnnotation> studyDesignDescriptors = new ArrayList<OntologyAnnotation>();
    @JsonProperty("protocols")
    public List<Protocol> protocols = new ArrayList<Protocol>();
}
```


Automatic conversion to/from ISA-JSON/ISA-TAB (under development)



Searchability



[Search](#) ▾ [Nanomaterials](#) ▾ [OpenTox](#) ▾ [Help](#) ▾

Welcome to eNanoMapper prototype database

A substance database for nanomaterial safety information

Search nanomaterials

Search, browse, upload

[Search nanomaterials
by identifier](#) ⓘ
[Search nanomaterials
by citation](#) ⓘ

[Search nanomaterials
by physchem
parameters or
biological effects](#) ⓘ

[Search nanomaterials
by composition](#) ⓘ

[Free text search](#) ⓘ

[Browse
nanomaterials and
studies](#) ⓘ
Data exchange via [REST](#)
[API](#) ↗ ⓘ

[Data import](#) ⓘ
Supported import formats:
OECD HT ⓘ, Excel
spreadsheets ⓘ


Help: Nanomaterials

The nanomaterials ⓘ are considered a special case of substances ⓘ. See [doi:10.3762/bjnano.6.165](https://doi.org/10.3762/bjnano.6.165) ↗.

eNanoMapper FP7 #604134. This project has received funding from the



Search by physchem and bio effects


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

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

Update results

▼ P-Chem

- ☐ 4.1. Appearance (S) [1]
- ☐ 4.26. Nanomaterial crystallite and grain size (S) [105]
- ☐ 4.27. Nanomaterial aspect ratio/shape (S) [9]
- ☐ 4.28. Nanomaterial specific surface area (S) [35]
- ☐ 4.29. Nanomaterial zeta potential (S) [249]
- ☐ 4.30. Nanomaterial surface chemistry (S) [368]
- ☐ 4.31. Nanomaterial dustiness (S) [1]
- ☒ 4.5. Particle size distribution (Granulometry) (S) [513]

Endpoint name Units

PARTICLE SIZE

Enter endpoint value

>= 50 <= 60

► Tox


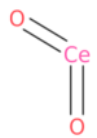
Update results

Hit list Download Help

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

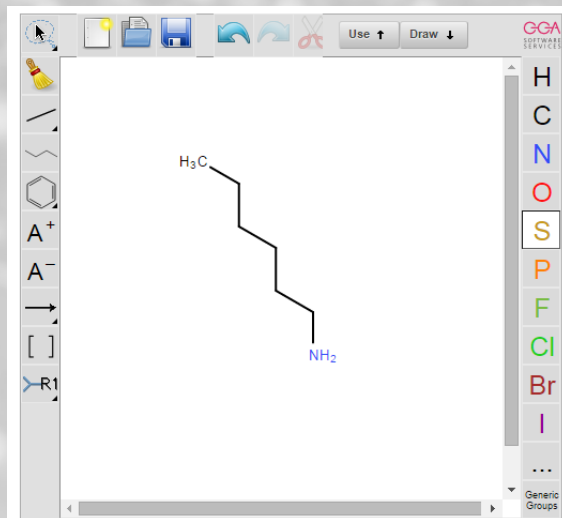
| | Substance Name | Substance UUID | Substance Type | Public name | Reference substance UUID | Owner | Info |
|--------------------------------|-----------------|----------------------------------|----------------|-------------|----------------------------------|--------------------------|--|
| <input type="checkbox"/> - 1 - | Limbach2005 NM1 | NWKI-7998492c... | ENM_9000006 | CeO2 I | NWKI-7998492c... | NanoWiki | Composition = CeO2 DATASET = NanoWiki Has_Identifier = 161 SOURCE = Limbach2005 |

Composition name:
Composition UUID: NWKI-7998492c-3902-3cc2-9f92-cdfe53cfc02
Purity of IUC Substance:

| Type | Name | EC No. | CAS No. | Typical concentration | Concentration ranges | Structure |
|------|--|--------|-----------|-----------------------|----------------------|---|
| Core |  CeO2 | | 1306-38-3 | 0 % (w/w) | 0 % (w/w) 0 % (w/w) | Also contained in...  |

Search:

Search by chemical composition



Chemical similarity is a pivotal concept in cheminformatics, encompassing a variety of computational methods quantifying the extent to which two chemical structures resemble each other.

There is not yet a standardized approach for NM similarity, however a number of attempts for NM grouping and read across have been published recently.

Search structures and associated data

Exact structure Similarity Substructure URL ☐ Filter by substance 0.5

Identifiers Datasets

Showing from 1 to 3 in pages of 20 entries

| | Diagram | CasRN | EC number | IUCLID 5 R | Names | Trade Name | IUPAC name | SMILES | Std. InChI key | Std. InChI | REACH registration date | Similarity |
|-------|---------|-------|-----------|------------|--|------------|------------|----------|----------------------------|-------------|-------------------------|------------|
| - 1 - | | | | FCSV-97... | Octadecylamine, octadecan-1-amine[REYJPSVUYRZGE-UHFFFAOYSA-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 | | | NCCCC... | REYJPSVUYRZGE-UHFFFAOYSA-N | InChI=1S... | | 0.72 |

Showing from 1 to 4 in pages of 20 substances

| | Substance Name | Substance UUID | Substance Type | Public name | Reference substance UUID | Coating | Contained in as |
|-------|----------------|----------------|----------------|-------------|--------------------------|--|-------------------------------------|
| - 1 - | S40.HDA | FCSV-0e... | NPO_1892 | S40.HDA | FCSV-9a... | Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv | Classification = Cationic coating 1 |
| - 2 - | G60.HDA | FCSV-ac... | NPO_401 | G60.HDA | FCSV-50... | Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv | Classification = Cationic coating 1 |
| - 3 - | G15.HDA | FCSV-c4f... | NPO_401 | G15.HDA | FCSV-50... | Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv | Classification = Cationic coating 1 |
| - 4 - | G30.DDT@HDA | FCSV-cb... | NPO_401 | G30.DDT@HDA | FCSV-50... | Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv | Classification = Cationic coating 1 |

| | | | | | | | | | | | | |
|-------|--|--|--|------------|-----------------------|--|--|----------|-----------------------------|-------------|--|------|
| - 3 - | | | | FCSV-0b... | 6-Amino-1-hexanethiol | | | NCCCC... | WYYXDSQOPIGZPU-UHFFFAOYSA-N | InChI=1S... | | 0.62 |
|-------|--|--|--|------------|-----------------------|--|--|----------|-----------------------------|-------------|--|------|



Substances / Materials representation

- **NanoParticle Ontology (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).
- **REACH Guidance:** “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.
- **IUPAC:** “Matter of constant composition best characterized by the entities (molecules, formula units, atoms) it is composed of. Physical properties such as density, refractive index, electric conductivity, melting point etc. characterize the chemical substance”

Material composition

| <div> </div> <div> Search Nanomaterials OpenTox Demo Help </div> | | | | | | | |
|--|--|-------------------|----------------|-----------------------|--------------------------|--|----------------------------|
| <div> Showing from 1 to 1 in pages of 10 substances Previous Next </div> <div>Filter...</div> | | | | | | | |
| | Substance Name | Substance UUID | Substance Type | Public name | Reference substance UUID | Owner | Info |
| - 1 - | G15.AC | FCSV-bc77c03d-... | nanoparticle | G15.AC | FCSV-50cca421-... | Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv | Classification = Anionic |
| <div> Composition name: Composition UUID: FCSV-bc77c03d-4e75-3fab-bb3d-17b983663819 Purity of IUC Substance: </div> | | | | | | | |
| Type | Name | EC No. | CAS No. | Typical concentration | Concentration ranges | | Structure |
| Coating | (2r)-2-Acetamido-3-Sulfanyl-Propanoic Acid,Pwskimoespyia-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 | [Au] | | | 0 % (w/w) | 0 % (w/w) | 0 % (w/w) | Also contained in... Au |

Coating

Core

Free text search supported by ontology annotated database

- Several technical options available

ENM eNanoMapper

Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

Free text search ☐ All ☒ Endpoint ☐ Protocol ☐ NM type

Substances Advanced search Download

Showing 15 entries (1 to 15)

| Term | Title | Related to | Hit relevance | Find studies |
|----------------|--------------------------------------|-----------------|---------------|--------------|
| NPO_1694 | PARTICLE SIZE.D90 | PC GRANULOMETRY | 65.103 | by endpoint |
| NPO_1694 | Core size | PC GRANULOMETRY | 55.203 | by endpoint |
| NPO_1617 | | | | |
| NPO_1694 | PARTICLE SIZE | PC GRANULOMETRY | 45.119 | by endpoint |
| NPO_1915 | Intensity Mean Hydrodynamic Diameter | PC GRANULOMETRY | 34.528 | by endpoint |
| NPO_1915 | Number Mean Hydrodynamic Diameter | PC GRANULOMETRY | 34.528 | by endpoint |
| NPO_1800 | | | | |
| NPO_1915 | Volume Mean Hydrodynamic Diameter | PC GRANULOMETRY | 34.528 | by endpoint |
| NPO_1800 | | | | |
| NPO_1915 | Z-Average Hydrodynamic Diameter | PC GRANULOMETRY | 23.676 | by endpoint |
| NPO_1916 | | | | |
| | Average Length | PC GRANULOMETRY | 10.044 | by endpoint |
| CHEMINF_000416 | Density | PC GRANULOMETRY | 10.044 | by endpoint |
| | Diameter | PC GRANULOMETRY | 10.044 | by endpoint |
| NPO_1915 | MASS MEDIAN AERODYNAMIC DIAMETER | PC GRANULOMETRY | 10.044 | by endpoint |
| | MASS MEDIAN DIAMETER | PC GRANULOMETRY | 10.044 | by endpoint |

Search for “metal oxide”

Endpoint ☐ Protocol ☒ NM type

| Related to | Hit relevance | Find studies |
|-------------|---------------|-------------------|
| ENM_9000006 | 12.363 | by substance type |
| NPO_1486 | 12.363 | by substance type |
| NPO_1542 | 12.363 | by substance type |
| NPO_1544 | 12.363 | by substance type |
| NPO_1548 | 12.043 | by substance type |
| NPO_1550 | 12.043 | by substance type |

Ontology supported free text search
UNDER DEVELOPMENT

Free text search ¹ with query expansion ¹ based on the eNanoMapper ontology and annotated database entries.

The results are sorted by hit relevance ¹.

The free text search finds ontology annotated database entries (e.g. protocols and endpoints in the second column).

The last column is a link leading to a list of studies.

Search for “size”

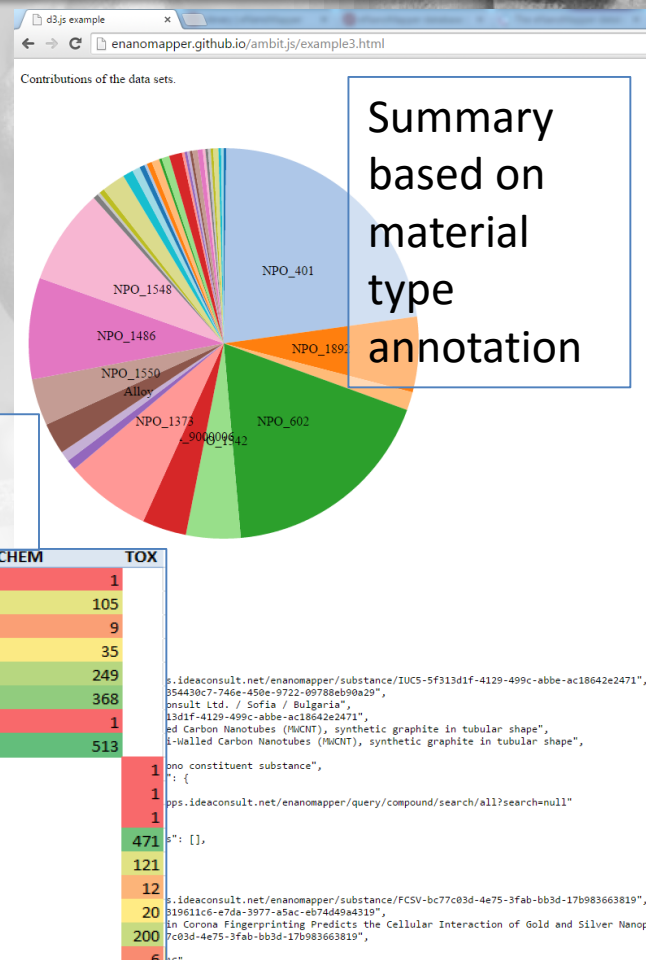
The search quality depends on ontology annotation

- How to annotate

- Data model supported (minimal)
- Manual annotation
- Parser supported annotation
- Automated heuristics

- Entries to be annotated

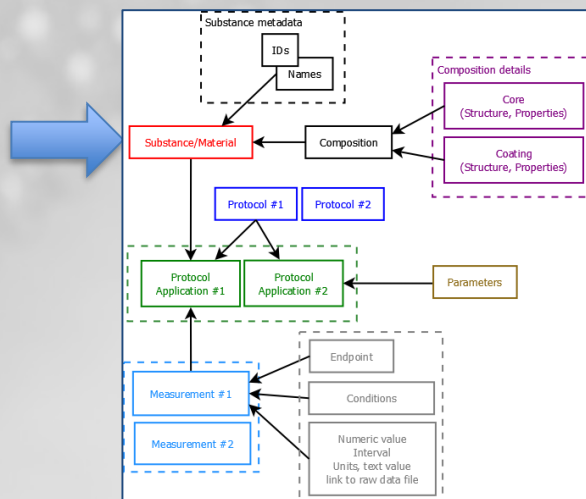
- Material types
- Assays
- Endpoints
- Protocol parameters
- Experiment factors
- Experiment results
- Units
- NM providers,
- NM identifiers, etc.



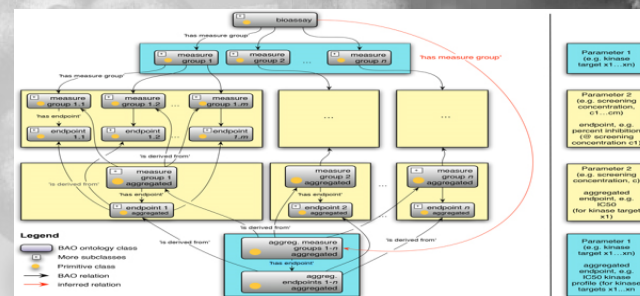
Comments welcome at
<https://github.com/enanomapper/data.enanomapper.net/issues/8>

Semantic search

Multiple
Input
formats



BioAssay Ontology



Semantic formats
RDF/XML
N3
JSON LD

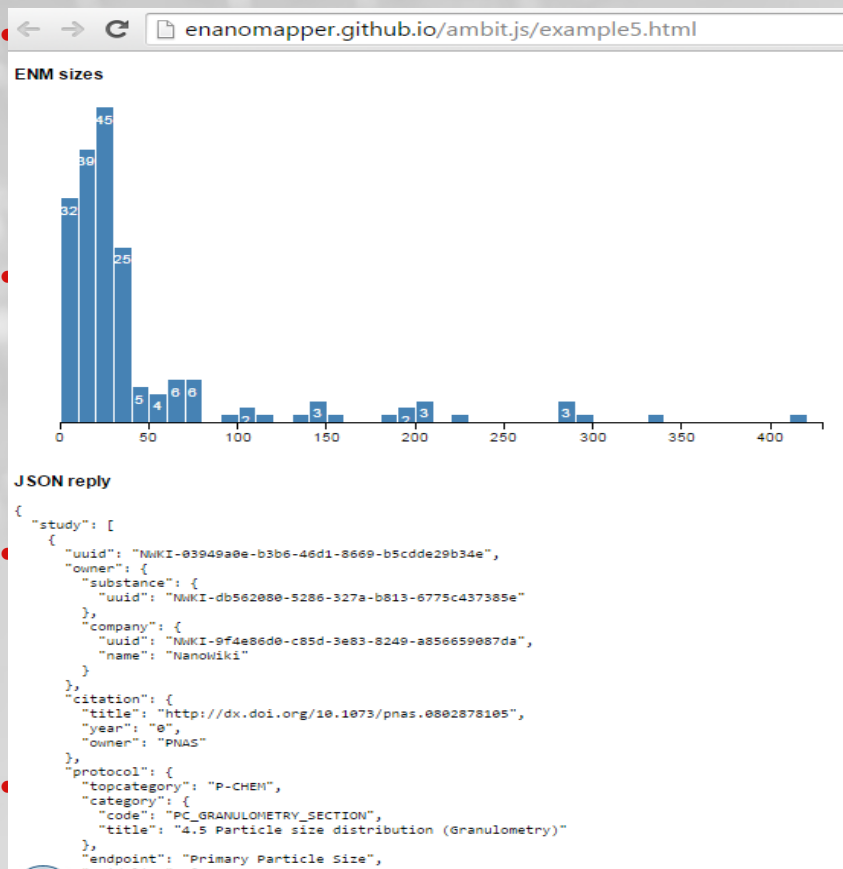
Triple store



Tailored interfaces

- Application Programming Interface (API)
- Use the API to
 - Develop user interface(s)
 - Communication with modelling tools
 - Integration with databases

eNanoMapper DB implementation : Application Programming Interface



- eNanoMapper database is based on the open source project

<http://ambit.sf.net>

ENM <https://apps.ideaconsult.net/enanomapper/api-docs> [Explore](#)

eNanoMapper prototype database API

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

| | |
|--|---|
| algorithm : OpenTox Algorithms service | Show/Hide List Operations Expand Operations Raw |
| bundle : Datasets of substances | Show/Hide List Operations Expand Operations Raw |
| compound : OpenTox Chemical Compounds service | Show/Hide List Operations Expand Operations Raw |
| dataset : OpenTox Dataset service | Show/Hide List Operations Expand Operations Raw |
| feature : OpenTox Feature service | Show/Hide List Operations Expand Operations Raw |
| model : OpenTox Prediction Models service | Show/Hide List Operations Expand Operations Raw |
| property : Chemical substances Properties service | Show/Hide List Operations Expand Operations Raw |
| query : Queries | Show/Hide List Operations Expand Operations Raw |
| compound : Chemical structures search | Show/Hide List Operations Expand Operations Raw |
| substance : Substance search | Show/Hide List Operations Expand Operations Raw |
| substance : Chemical Substances service | Show/Hide List Operations Expand Operations Raw |
| GET /substance | List substances |
| POST /substance | Import substance(s) and studies |
| GET /substance/{uuid} | Get a substance |
| GET /substance/{uuid}/composition | Get substance composition |
| GET /substance/{uuid}/structures | Get substance composition as a dataset |
| GET /substance/{uuid}/study | Get substance study |
| GET /substance/{uuid}/studysummary | Get study summary for the substance |
| substanceowner : Substance owners | Show/Hide List Operations Expand Operations Raw |
| task : OpenTox Task service (asynchronous jobs) | Show/Hide List Operations Expand Operations Raw |

[BASE URL: <https://apps.ideaconsult.net/enanomapper/api-docs> , API VERSION: 2.7.2]

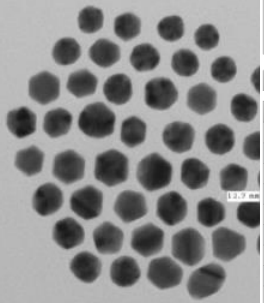
<http://enanomapper.github.io/API/>



culations (uses API to
d store back results)

s using MOPAC

-



[Home](#) \ [Datasets](#) \ [Dataset browser](#) \ https://apps.ideaconsult.net/enmtest/dataset/39?feature_uris...

[Identifiers](#) | [Names](#) | [Calculated](#) | [Other](#)

☒ NO. OF FILLED LEVELS ⓘ
 ☒ TOTAL ENERGY ⓘ
 ☒ FINAL HEAT OF FORMATION ⓘ
 ☒ IONIZATION POTENTIAL ⓘ
 ☒ ELECTRONIC ENERGY ⓘ

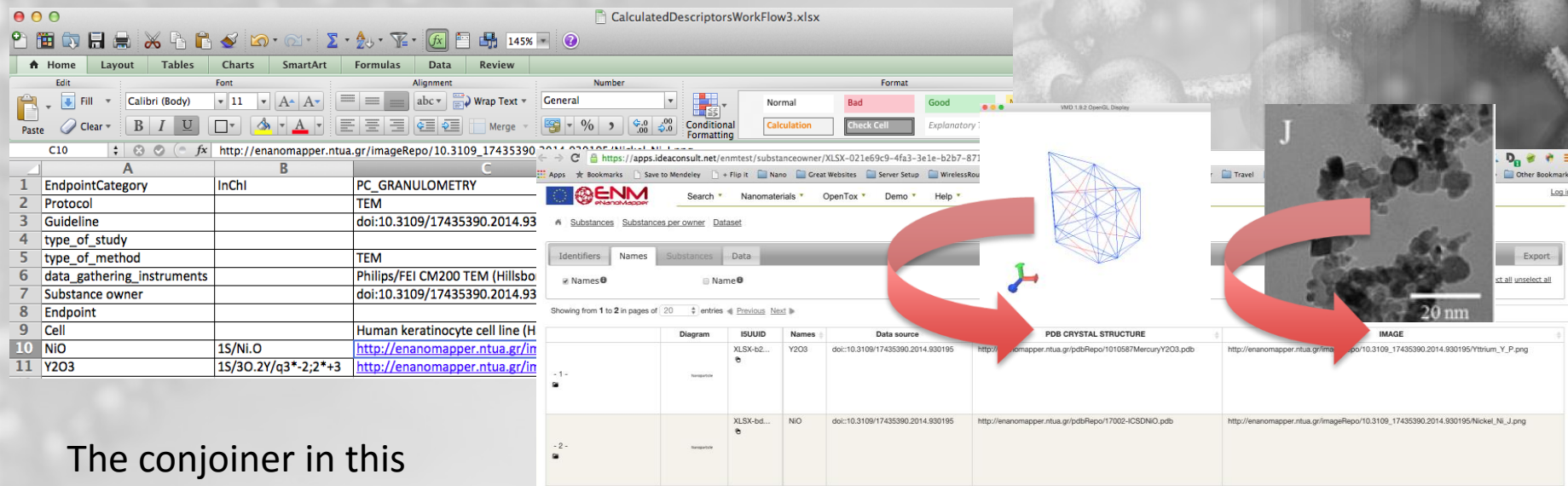
☒ CORE-CORE REPULSION ⓘ
 ☒ MOLECULAR WEIGHT ⓘ
 ☒ EHOMO ⓘ
 ☒ ELUMO ⓘ

Showing from 1 to 1 in pages of 20 entries
[Previous](#)
[Next](#)

| | Diagram | NO. OF FILLED LEVELS ⓘ | TOTAL ENERGY ⓘ | FINAL HEAT OF FORMATION ⓘ | IONIZATION POTENTIAL ⓘ | ELECTRONIC ENERGY ⓘ | CORE-CORE REPULSION ⓘ |
|-------|---------|------------------------|----------------|---------------------------|------------------------|---------------------|-----------------------|
| - 1 - | | 88 | -7060.669 | 1672.661 | 3.898 | -59148.238 | 52087.566 |

| | | | | | |
|----|-----|-----|---------|-------|--|
| 9 | 626 | 100 | 92.083 | 0.928 | <input checked="" type="checkbox"/> Minor |
| 10 | 790 | 100 | 103.983 | 0.918 | <input checked="" type="checkbox"/> Major |
| 11 | 787 | 100 | 105.397 | 0.890 | <input checked="" type="checkbox"/> Integrated Density |
| 12 | 969 | 100 | 115.640 | 0.911 | <input checked="" type="checkbox"/> Kurtosis |

WP4: A service to transform the data into ready-to-model-form



The screenshot displays the eNanoMapper workflow interface. On the left, a spreadsheet titled 'CalculatedDescriptorsWorkflow3.xlsx' shows input data for a substance. The data is then processed through a series of steps, including 'Identifiers', 'Names', 'Substances', and 'Data'. The final output is a dataset ready for modeling, which includes a table of substances and their associated data sources.

| Diagram | ISUID | Names | Data source | PDB CRYSTAL STRUCTURE | IMAGE |
|------------|-------|----------------------------------|---|--|-------|
| XLSX-b2... | Y203 | doi:10.3109/17435390.2014.930195 | http://enanomapper.ntua.gr/pdbRepo/1010587MercuryY203.pdb | http://enanomapper.ntua.gr/imageRepo/10.3109_17435390.2014.930195Yttrium_Y_P.png | |
| XLSX-bd... | NiO | doi:10.3109/17435390.2014.930195 | http://enanomapper.ntua.gr/pdbRepo/17002-ICSDNiO.pdb | http://enanomapper.ntua.gr/imageRepo/10.3109_17435390.2014.930195Nickel_Ni_J.png | |

The conjoiner in this example converts heterogeneous data of metal oxides (image and crystal structure) into a dataset ready for modeling.

compound:

```
{
  URI: "https://apps.ideaconsult.net/enmtest/substance/XLSX-b2a6a8e9-a7d4-349c-9fcc-df05356a508d"
},
```

values:

```
{
  http://app.jaqpot.org:8080/jaqpot/services/feature/image+average+particle+angle: 149.23083,
  http://app.jaqpot.org:8080/jaqpot/services/feature/image+average+particle+area: 8803,
  http://app.jaqpot.org:8080/jaqpot/services/feature/image+average+particle+area_fraction: 43.979816,
  http://app.jaqpot.org:8080/jaqpot/services/feature/image+average+particle+aspect_ratio: 1.3006951,
  http://app.jaqpot.org:8080/jaqpot/services/feature/image+average+particle+circularity: 0.34530884,
```



The need of integration ... is not unique for nanomaterials

- 2005: “Integrated Informatics in Life and Materials Sciences: An Oxymoron?” *
 - Calculations, Descriptors, Statistics, Models
 - Data (substances, chemical structures, properties, predictions)
- Approaches toward integration:
 - Workflow management systems
 - Standalone container applications (chassis)
 - Web services, web mashups
 - Index –time integration vs query-time integration

* *Gilardoni, F., Curcin, V., Karunanayake, K., Norgaard, J., & Guo, Y. (2005). QSAR Combinatorial Science, 24(1), 120-130.*

Chemical /Toxicogenomics DB

(no explicit NM support)



ChEMBL



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

HTML, REST API, Bulk download

NM: Fullerenes , Metal oxides

HTML, REST API, Bulk download

Gene expression data

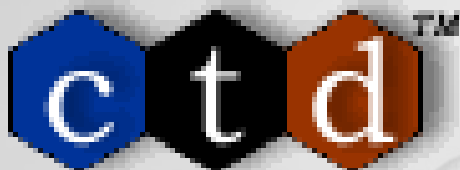
NM: carbon nanotubes, quantum dots, graphene oxide, zinc oxide, silver and gold nanoparticles.

HTML, REST API, Bulk download

Comparative Toxicogenomics Database

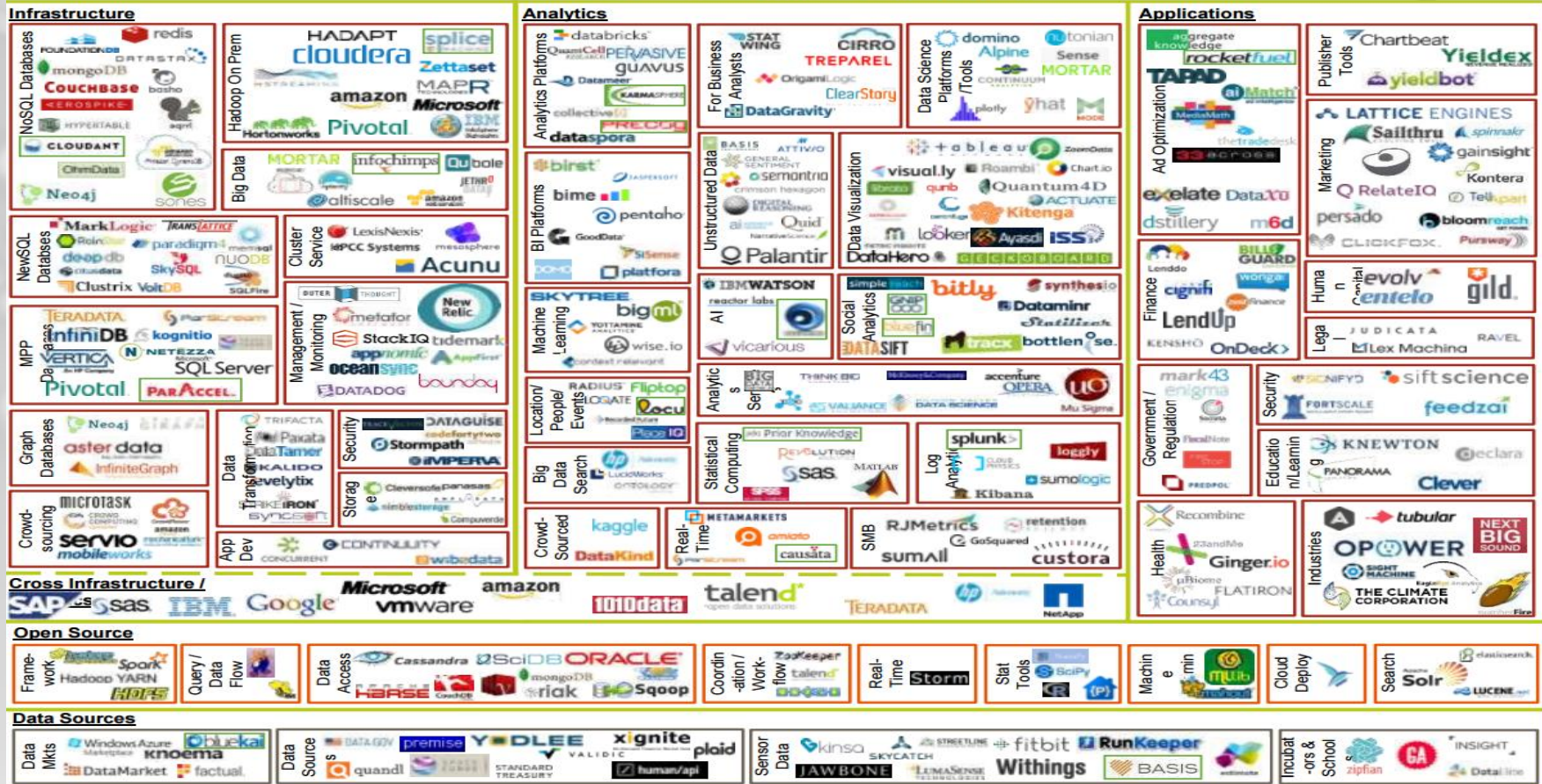
Includes nanomaterial related data. **HTML**

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



Data management and analytics

BIG DATA LANDSCAPE, VERSION 3.0



© Matt Turck (@mattturck), Sutian Dong (@sutiandong) & FirstMark Capital (@firstmarkcap)



Data integration options

- Databases A & B
- Match entities
 - Common data model
 - Distinct data models, links
 - Distinct data models, joins
- Retrieve query results
 - Index time merging
 - Query time merging
 - Hybrid - Where practical, content is indexed centrally. Repositories for which this is not cost effective (or simply not possible) are federated to at query time.

| | Single storage | Separate storage |
|----------------------|-------------------------------|---|
| Common data model | <i>Typical data warehouse</i> | <i>WWW</i> |
| Distinct data models | <i>Data lake</i> | <i>Toxygates *</i> <i>(2013)</i> <i>EMBL-EBI RDF</i> <i>** Platform</i> <i>(2013)</i> |

* <http://toxygates.nibio.go.jp/>

** <http://www.ebi.ac.uk/rdf/>

A **data lake** is a large storage repository and processing engine. They provide "massive storage for any kind of data, enormous processing power and the ability to handle virtually limitless concurrent tasks or jobs"

Identifiers for materials and measurements

- No unique identifiers for NM
 - Note “*Substance Identification*” is also an issue for chemicals in REACH
- However
 - NM are composed of chemical structures (hence identifiers available)
 - Crystallography , material structure
 - NM specific categorization exist (e.g. NanoCarbon nomenclature)
 - Measurements, protocols, endpoints, instruments, assay conditions – annotate by ontology entries



TOOLS AVAILABLE

2 February 2016



data.enanmapper.net



Search ▾ Nanomaterials ▾ OpenTox ▾ Help ▾

Nanomaterial bundles

Download

Help

| Title ▾ | Version ▾ | Code ▾ | Status ▾ |
|--|-----------|---|----------------------|
| Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles | 1 | 10.1021/nn406018q | draft |
| OECD Harmonized Templates import test | 1 | Multi-Walled Carbon Nanotubes (MWCNT), synthetic graphite in tubular shape | draft |
| NanoWiki | 1 | NanoWiki | published |
| In Vitro data from FP7 MARINA project (KI) | 1 | Comprehensive In Vitro Toxicity Testing of a Panel of Representative Oxide Nanomaterials: First Steps towards an Intelligent Testing Strategy | published enanmapper |

Protein Corona database

MWCNT

NANOWIKI

FP7 MARINA/ KI

This is a demonstration.
The data from the community allows to validate the approach of reconciliation of multiple formats into the same data model, while providing search and supporting data analysis

[00000000-0000-0000-0000-000000000001](#)



[91cad054-4de8-4dc9-a8e4-20564e7eada7](#)



eNanoMapper data model

- **Flexible**
 - General structure to describe measurements, but NO fixed fields for endpoints, experiment conditions, etc.
- **Fields annotated by ontology entries**
- **Allows conversion between different formats and data models**
 - Necessary for data integration!
- **Programmatic access (API)**
 - i.e. support for data analysis
- **User friendly interface**
 - Consuming the API (e.g. JavaScript)

eNM data model = generic description of any measurement. Does not specify what to record to describe particular experiment.


- The later is a domain specific scientific question
- Related work: CoDATA UDS , zeta potential pilot by US NanoWG, OECD WPMN, the NanoSafety cluster templates

How to represent the selected “aspects of the reality” in a database or ontology is a data representation question

- Computer science, logic, data modelling; informed by the expected usage



Format conversions, ISA schema

x  <https://github.com/enanomapper/nmdataparser>

The **nmdataparser** Java library is a configurable parser allowing to importing spreadsheet substance composition, characterisation and assay data into the **eNanoMapper database**, via [\[API\]](#). The parser converts the spreadsheet into the internal **AMBIT** data model, using a JSON file for mapping the objects. The main class `GenericExcelParser` iterates over entries of `*.xls` and `*.xlsx` files returning a set of `SubstanceRecords` objects.

N. Jeliaskova, C. Chomenidis, P. Doganis, B. Fadeel, R. Grafström, B. Hardy, J. Hastings, M. Hegi, V. Jeliaskov, N. Kochev, P. Kohonen, C. R. Munteanu, H. Sarimveis, B. Smeets, P. Sopasakis, G. Tsiliki, D. Vorgrimmmler, and E. Willighagen, The eNanoMapper database for nanomaterial safety information, *Beilstein J. Nanotechnol.*, vol. 6, pp. 1609-1634, Jul. 2015. [doi:10.3762/bjnano.6.165](#)

Support for ISA-TAB / ISA-JSON pending

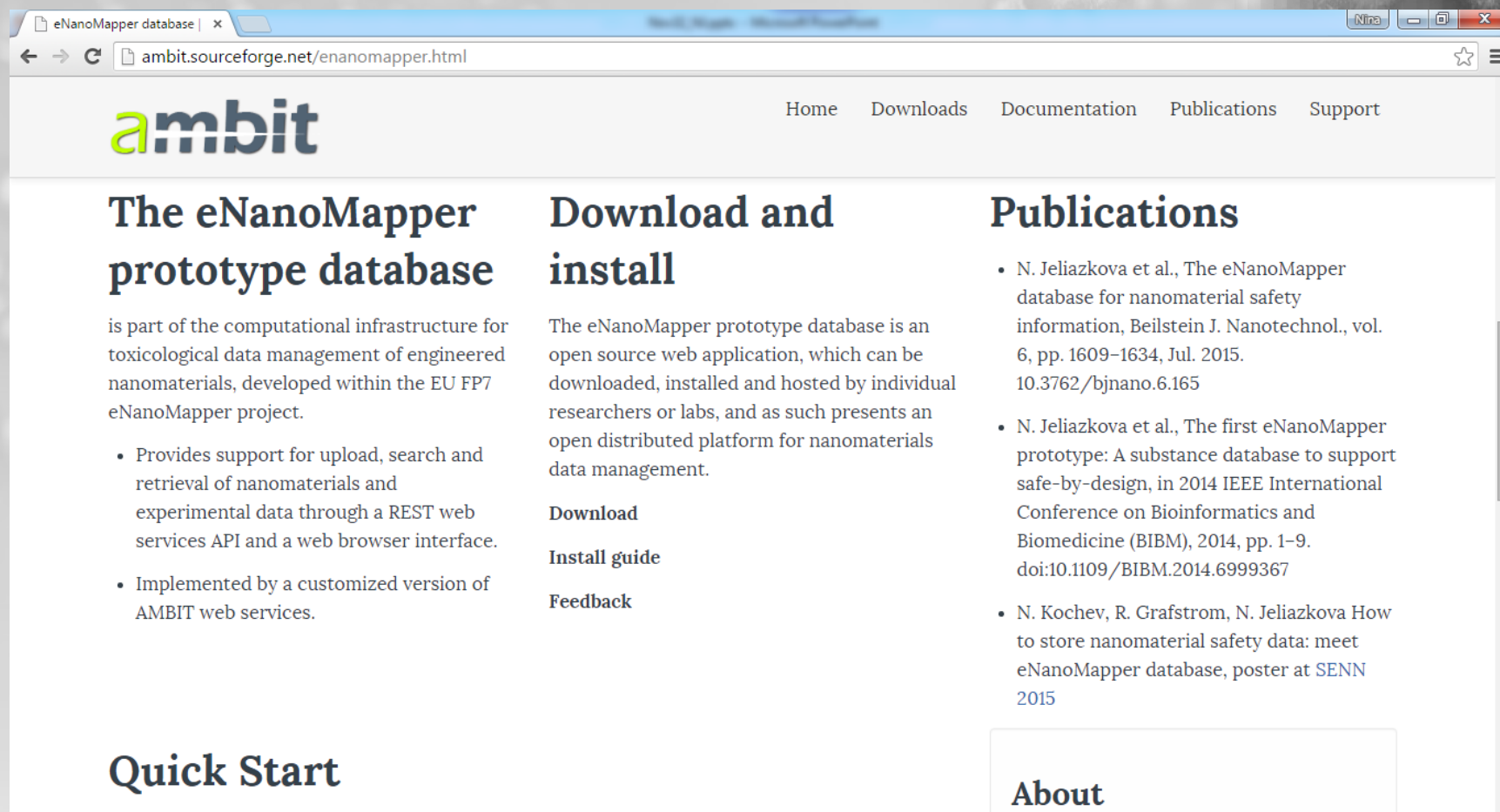
Stable release [DOI 10.5281/zenodo.34065](#)

```
<dependency>
  <groupId>net.enanomapper</groupId>
  <artifactId>nmparser</artifactId>
  <version>1.0.0</version>
</dependency>
```

Open source,
available at GitHub



Downloadable



The screenshot shows a web browser window with the address bar displaying "ambit.sourceforge.net/enanomap.html". The website has a navigation bar with links: Home, Downloads, Documentation, Publications, and Support. The main content area is divided into three columns. The left column is titled "The eNanoMapper prototype database" and describes it as part of a computational infrastructure for toxicological data management, developed within the EU FP7 eNanoMapper project. It lists two bullet points: "Provides support for upload, search and retrieval of nanomaterials and experimental data through a REST web services API and a web browser interface." and "Implemented by a customized version of AMBIT web services." Below this is a "Quick Start" section. The middle column is titled "Download and install" and describes the eNanoMapper prototype database as an open source web application that can be downloaded, installed, and hosted by individual researchers or labs, and as such presents an open distributed platform for nanomaterials data management. It includes links for "Download", "Install guide", and "Feedback". The right column is titled "Publications" and lists three references: 1. N. Jeliaskova et al., The eNanoMapper database for nanomaterial safety information, Beilstein J. Nanotechnol., vol. 6, pp. 1609-1634, Jul. 2015. doi:10.3762/bjnano.6.165. 2. N. Jeliaskova et al., The first eNanoMapper prototype: A substance database to support safe-by-design, in 2014 IEEE International Conference on Bioinformatics and Biomedicine (BIBM), 2014, pp. 1-9. doi:10.1109/BIBM.2014.6999367. 3. N. Kochev, R. Grafstrom, N. Jeliaskova How to store nanomaterial safety data: meet eNanoMapper database, poster at SENN 2015. Below the publications is an "About" section.

ambit

Home Downloads Documentation Publications Support

The eNanoMapper prototype database

is part of the computational infrastructure for toxicological data management of engineered nanomaterials, developed within the EU FP7 eNanoMapper project.

- Provides support for upload, search and retrieval of nanomaterials and experimental data through a REST web services API and a web browser interface.
- Implemented by a customized version of AMBIT web services.

Quick Start

Download and install

The eNanoMapper prototype database is an open source web application, which can be downloaded, installed and hosted by individual researchers or labs, and as such presents an open distributed platform for nanomaterials data management.

Download

Install guide

Feedback

Publications

- N. Jeliaskova et al., The eNanoMapper database for nanomaterial safety information, Beilstein J. Nanotechnol., vol. 6, pp. 1609-1634, Jul. 2015. doi:10.3762/bjnano.6.165
- N. Jeliaskova et al., The first eNanoMapper prototype: A substance database to support safe-by-design, in 2014 IEEE International Conference on Bioinformatics and Biomedicine (BIBM), 2014, pp. 1-9. doi:10.1109/BIBM.2014.6999367
- N. Kochev, R. Grafstrom, N. Jeliaskova How to store nanomaterial safety data: meet eNanoMapper database, poster at SENN 2015

About



Published

□ N. Jeliaskova, et al. "The eNanoMapper database for nanomaterial safety information," *Beilstein J. Nanotechnol.*, vol. 6, pp. 1609–1634, Jul. 2015.

□ N. Jeliaskova, et al. "The first eNanoMapper prototype: A substance database to support safe-by-design," in *2014 IEEE International Conference on Bioinformatics and Biomedicine (BIBM)*, 2014, pp. 1–9.

The screenshot displays the Beilstein Journal of Nanotechnology website. The URL in the browser is beilstein-journals.org/bjnano/single/articleFullText.htm?publicId=2190-4286-6-165. The page features the journal's logo and title at the top. A navigation bar includes links for HOME, SUBMISSION, HELP, and an ADVANCED SEARCH button. On the left, there are sections for BROWSE (Thematic Series, All Volumes, Latest Articles, Most Accessed, Authors) and GO TO ARTICLE (Volume and No./Pages dropdowns). Below this is an EXCLUSIVE section for Beilstein Magazine, which is an open access publication presenting essays and other contributions from leading scientists. The main content area displays the article title "The eNanoMapper database for nanomaterial safety information" by Nina Jeliaskova¹, Charalampos Chomenidis², Philip Doganis², Bengt Fadeel³, Roland Grafström³, Barry Hardy⁴, Janna Hastings⁵, Markus Hegi⁴, Vedrin Jeliaskov¹, Nikolay Kochev^{1,6}, Pekka Kohonen³, Cristian R. Munteanu^{7,8}, Haralambos Sarimveis², Bart Smeets⁷, Pantelis Sopasakis^{2,9}, Georgia Tsiliki², David Vorgrimmler¹⁰ and Egon Willighagen⁷. The article is part of the Thematic Series "Nanoinformatics for environmental health and biomedicine". The guest editor is R. Liu. The article was received on 31 Mar 2015, accepted on 03 Jul 2015, and published on 27 Jul 2015. The full research paper is available. The abstract states: "Background: The NanoSafety Cluster, a cluster of projects funded by the European Commission, identified the need for a computational infrastructure for toxicological data management of engineered nanomaterials (ENMs). Ontologies, open standards, and interoperable designs were envisioned to empower a harmonized approach to European research in nanotechnology. This setting provides a number of opportunities and challenges in the".



More details on eNanoMapper?

For any additional information, please ask us
or download our publicly available Deliverables.


Douglas Connect
Working communities



in silico toxicology

IOFA
consult



EMBL-EBI 



misvik biology 

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Questions?

THANK YOU!