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Nanotechnology Working Group
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Comprehensively curated, validated data on a scale suitable for decision making

Web Address: www.nanomaterialregistry.org
Minimal Information about Nanomaterials (MIAN)

**DOMAIN:** CHARACTERIZATION + STUDY DATA

- **Property Measurements:** Material and system properties.
- **Ecological:** Impact on the natural environment.
- **Medical:** Drug delivery, nanomedicine applications.
- **Toxicology:** Potential toxicity of nanomaterials.

- **Validated** both programatically and by a team of scientists.
- **Integrated** through controlled vocabulary and data formatting.
- **Relevant** growing body of data that is available to the public.

**Reference Materials:** Benchmark Data.

**Meta Data:** The data about the data.

**Meta Data:** The data about the data.
A controlled vocabulary of PCC & measurands have been identified (https://www.nanomaterialregistry.com/resources/Glossary.aspx)
The Nanomaterial Registry’s **COMPLIANCE LEVEL FEATURE** provides a **METRIC** on the **QUALITY** of characterization of a nanomaterial record.

### Compliance Levels

<table>
<thead>
<tr>
<th>Compliance Level</th>
<th>Score</th>
<th>Medal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gold</td>
<td>76-100</td>
<td>🌟</td>
</tr>
<tr>
<td>Silver</td>
<td>51-75</td>
<td>🏆</td>
</tr>
<tr>
<td>Bronze</td>
<td>26-50</td>
<td>🏆</td>
</tr>
<tr>
<td>Merit</td>
<td>0-25</td>
<td>🏆</td>
</tr>
</tbody>
</table>

**COMPLIANCE LEVELS** are broken into **MERIT**, **BRONZE**, **SILVER**, and **GOLD** and represent increasing quality of characterization based on our evaluation criteria.

**A COMPLIANCE LEVEL SCORE** is a quantitative value calculated by an algorithm.

**MORE INFORMATION:**
https://www.nanomaterialregistry.com/about/HowIsComplianceCalculated.aspx
How do you get data?

The Nanomaterial Registry’s DATA are manually curated by lab-trained nanomaterial scientists.

In the Past: Data have been received through public databases, manufacturer catalogs, or through data partnerships (received in pdf papers or reports)

Current Movement: Create and adopt data submission template
- Excel format
- Matching the MIAN categories
- Submission online

Investigating the use of NIST’s Materials Data Curation System (XML format)
ISA-Tab-Nano will also be linked as a resource, but it is not automatic upload at this time
Web Address: www.nanomaterialregistry.org
### DATA QUALITY METRIC

<table>
<thead>
<tr>
<th>Scenario 1</th>
<th>Scenario 2</th>
<th>Scenario 2</th>
<th>Scenario 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Size= 37.5 nm</td>
<td>Size= 37.5 nm</td>
<td>Size= 37.5 nm</td>
<td>Size= 37.5 nm</td>
</tr>
<tr>
<td>Mean Hydrodynamic Diameter</td>
<td>Mean Hydrodynamic Diameter</td>
<td>Dynamic Light Scattering</td>
<td>Dynamic Light Scattering</td>
</tr>
<tr>
<td>Malvern ZetaSizer Nano ZS</td>
<td>Malvern ZetaSizer Nano ZS</td>
<td>11 of 12 measurement parameters reported</td>
<td>Protocol: ASTM E2490 - 09</td>
</tr>
</tbody>
</table>

**Algorithm**

Assigns weights to each value in a curated record

\[
CL_{PCC} = \sum_{Measurements} \left( \frac{\sum G M_G * P_G}{\sum G M_G * W_G} \right)
\]

[https://www.nanomaterialregistry.com/about/HowIsComplianceCalculated.aspx](https://www.nanomaterialregistry.com/about/HowIsComplianceCalculated.aspx)
Nanomaterial Registry

DATA ANALYSIS @ nanoHUB
The Nanomaterial Registry offers a data export that focuses on nanomaterial characterization data. This is currently a limitation on the questions users can ask of the Registry’s data.
Valuable partnership with nanoHUB
1. The Registry’s own website is designed for use as a reference library
2. nanoHUB offers data handling that appeals to the predictive modeling community

nanoHUB received an NSF stipend to participate in case studies of data hosting with RTI International (Nanomaterial Registry) and the Center for the Environmental Implications of NanoTechnology (CEINT) at Duke University

Registry Portal is now available and offers the Nanomaterial Registry’s authoritatively-curated data in a format useful for sorting and filtering by modeling researchers

https://nanohub.org/groups/nanomaterialregistry
Nanomaterial data records with associated bio/env assay studies were exported from the Nanomaterial Registry and uploaded to the Registry Portal at nanoHUB.

Assertion terms can be selected to build your data subset.
Nanomaterial data records with associated bio/env assay studies were exported from the Nanomaterial Registry and uploaded to the Registry Portal at nanoHUB.

- Data are presented in a spreadsheet style for easy sorting and filtering
- Data can also be exported
NANOMATERIAL REGISTRY PORTAL

Data visualizations available at this time:

- Bar chart
- Heat map

Custom columns can be created with the help of data visualizations.
NANOMATERIAL REGISTRY PORTAL

The Registry portal can be reached from the Registry homepage or by searching for the Nanomaterial Registry at nanoHUB’s website.

www.nanomaterialregistry.org
STATE OF THE SCIENCE

Evolving Registry and Tools

- Gap Filling
- Decision Making

Enter new data into the Registry

Search

Answer

Design Experiments

Inference

NANOMATERIAL REGISTRY
LINKING AND SHARING INFORMATION

- **Ontology/Taxonomy**: Create data linkages and provide users with the ability to retrieve information.

- **User Interface**: Provide guidance to end users without backend complexity, share information.

- **Sustainable Data**: Build and validate applications.

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NANO MATERIAL REGISTRY
DATA SHARING

Data and Metadata shared in a public repository

- Research Motivated
  - Easy-to-use tools
  - Particular goals of collaboration

- Journal Requirement
  - Journals need convincing

- Funding Requirement
  - Understand the ROI
“Beginning in January 2015, we will start asking authors of all life sciences submissions that are sent out for peer review to complete relevant portions of the same checklist (available at http://www.nature.com/authors/policies/checklist.pdf), and will make the document available to referees during review.”
Nanomaterial Registry as an important tool for compliance with the NIH Data Sharing Policy

Department of Health and Human Services Part 1. Overview Information

Funding Opportunity Title
Centers of Cancer Nanotechnology Excellence (CCNE) (U54)

Funding Opportunity Announcement (FOA) Number: RFA-CA-14-013

The applicants are encouraged to consider using, as appropriate, various relevant NCI-supported resources described below.

Nanotechnology-related informatics.

... NCI supports the Nanomaterial Registry (https://www.nanomaterialregistry.org/), which archives research data on nanomaterials and their biological and environmental implications from a broad collection of publically available nanomaterial resources.
NANOMATERIAL REGISTRY

Thank You!

www.nanomaterialregistry.org
nanoregistry@rti.org

Select Project Publications


