

# NANOMATERIALREGISTRY

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Nanotechnology Working Group

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# NANOMATERIALREGISTRY



*Comprehensively  
curated, validated data  
on a scale suitable for  
decision making*

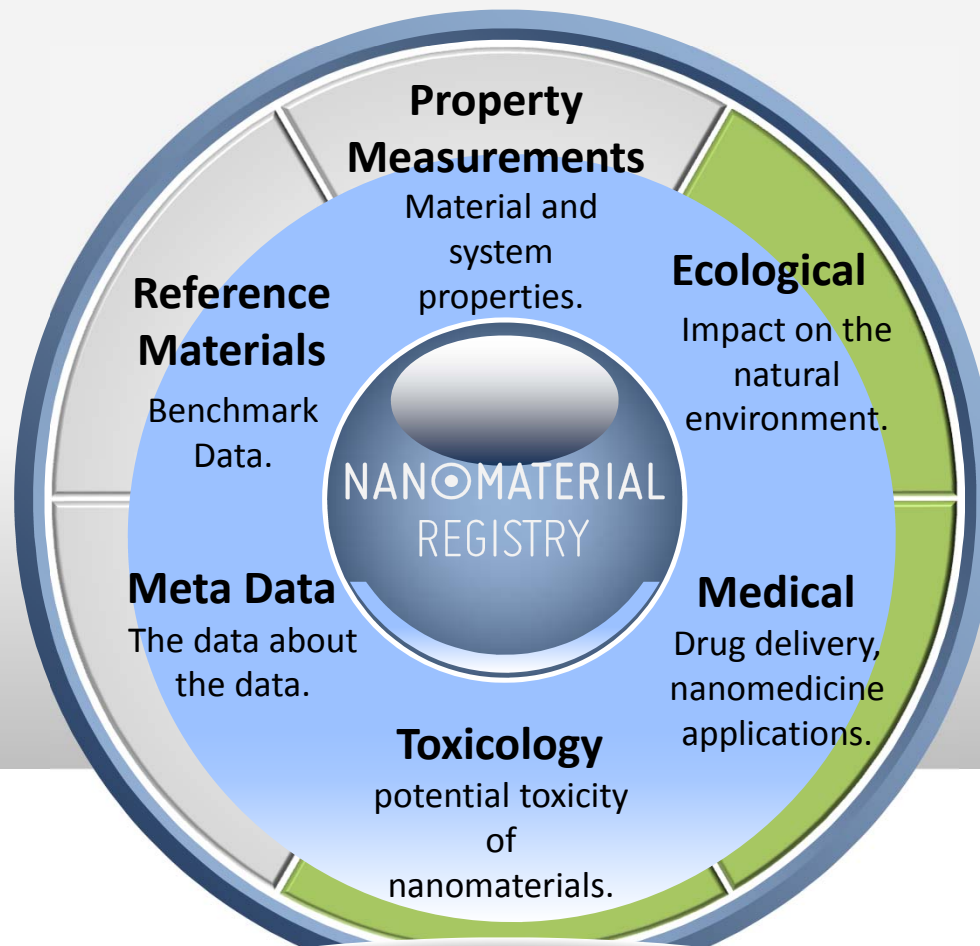
The screenshot shows the homepage of the Nanomaterial Registry. At the top, there is a navigation bar with links for 'ABOUT THE REGISTRY', 'RESOURCES', and 'CONTACT US', along with a search bar and social media icons. The main header features a large image of nanomaterials with the text 'WELCOME TO THE NANOMATERIAL REGISTRY!' and a brief description of the registry's purpose. Below this is a navigation menu with categories like 'Nanomaterial Registry', 'Data Export', 'Need Data Management?', 'Compliance Levels', 'Instance of Characterization', and 'Minimal Information About Nanomaterials'. The main content area is divided into three columns: 'BROWSE NANOMATERIALS' with filters for Material Type, Size, Shape, and Surface Area; 'A TOOL FOR THE NANOMATERIAL COMMUNITY' with a paragraph about the registry's mission and a 'Funded by:' section listing the NIH and National Institutes of Health; and 'LATEST NEWS' with two news items from August 2014.

**Web Address:**

**www.nanomaterialregistry.org**

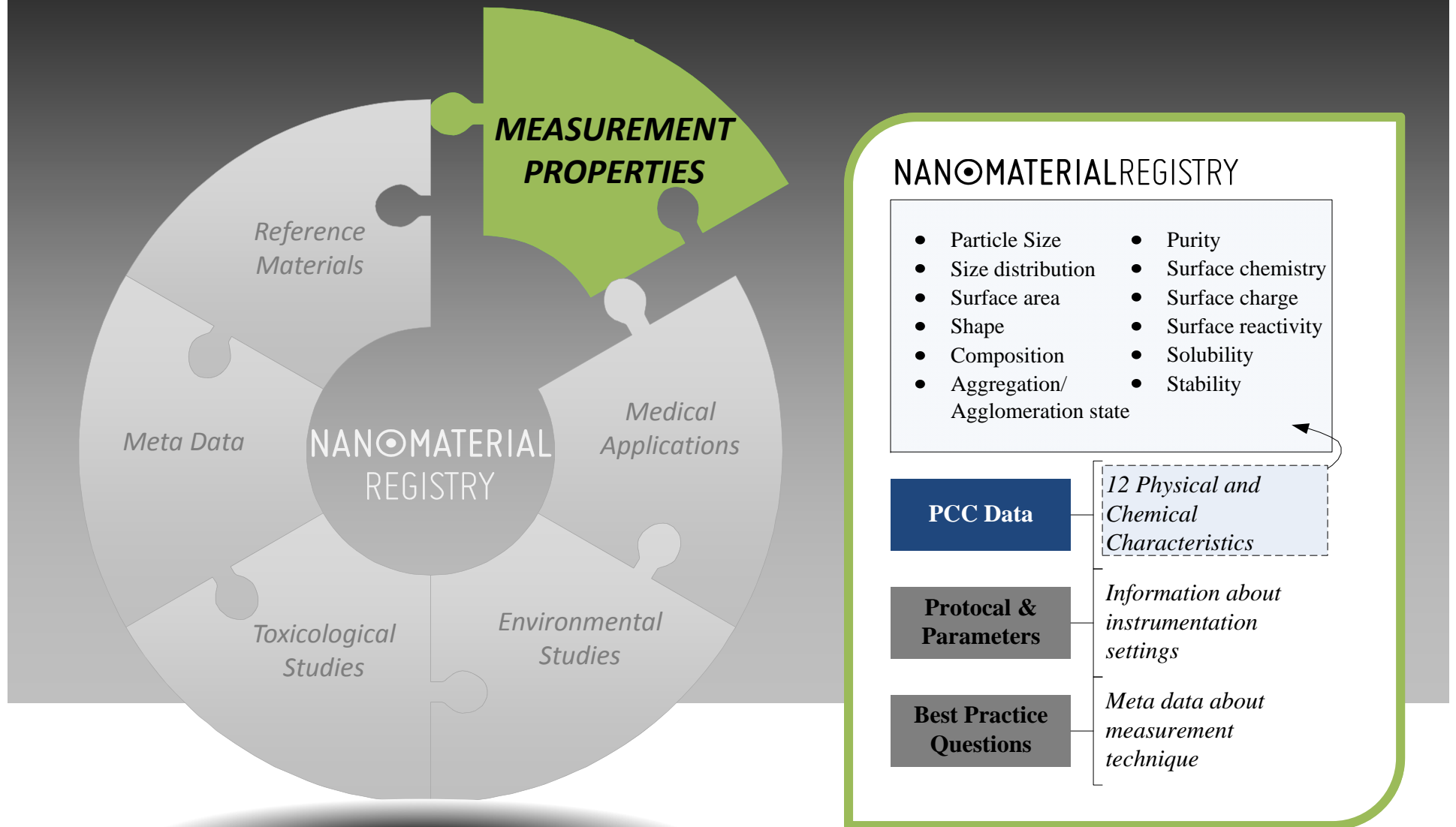
# Minimal Information about Nanomaterials (MIAN)

**DOMAIN:** CHARACTERIZATION + STUDY DATA



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

# Minimal Information about Nanomaterials (MIAN)







A **controlled vocabulary** of PCC & measurands have been identified (<https://www.nanomaterialregistry.com/resources/Glossary.aspx>)

# DATA QUALITY METRIC



The Nanomaterial Registry's **COMPLIANCE LEVEL FEATURE** provides a **METRIC** on the **QUALITY** of characterization of a nanomaterial record

Compliance Level	Score	Medal
Gold	76-100	
Silver	51-75	
Bronze	26-50	
Merit	0-25	

**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>

# DATA ACQUISITION

## How do you get data?

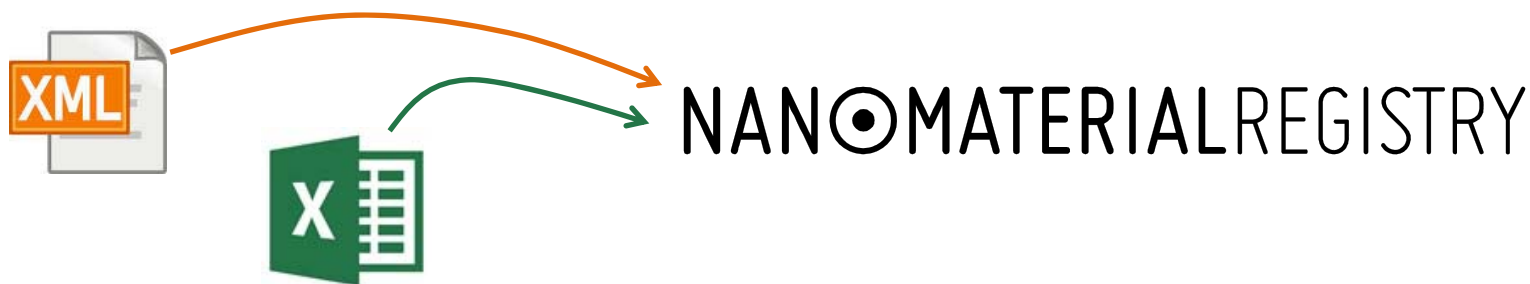
The Nanomaterial Registry's **DATA** are manually curated by lab-trained nanomaterial scientists.

*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

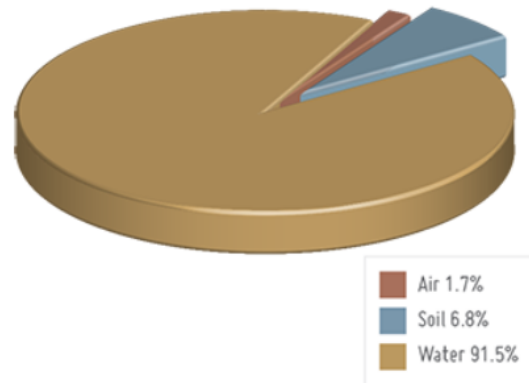
*Investigating the use of NIST's Materials Data Curation System (XML format)  
ISA-Tab-Nano will also be linked as a resource, but it is not automatic upload at this time*



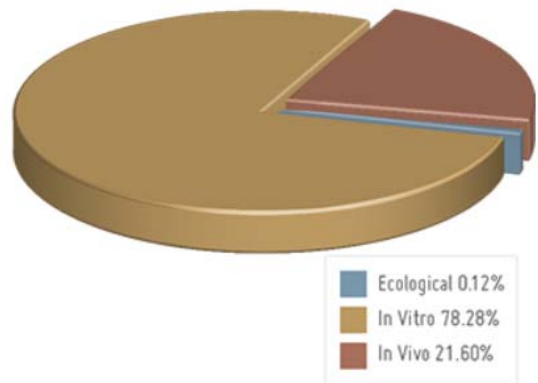
# NANOMATERIALREGISTRY



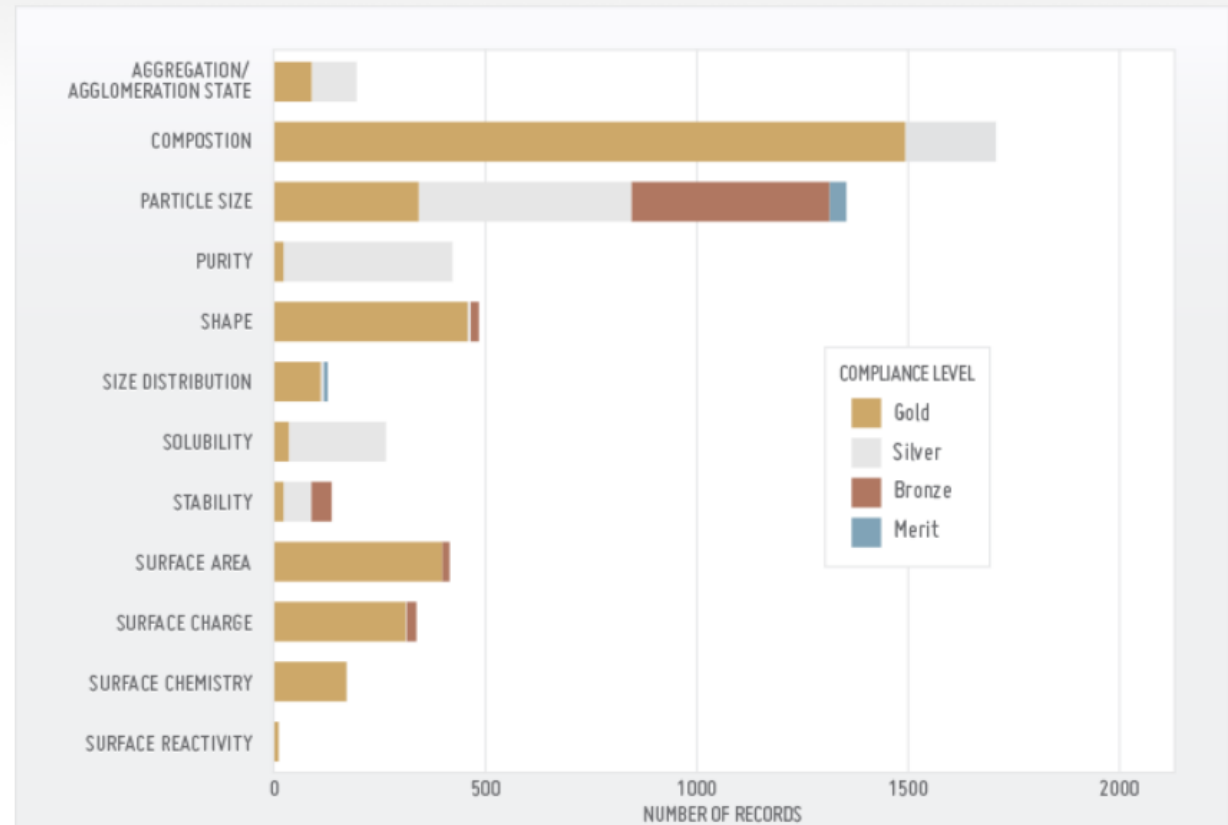
Environmental Studies (59 total)



Biological Studies (819 total)



Characterization Profile for Nanomaterials



Web Address:

[www.nanomaterialregistry.org](http://www.nanomaterialregistry.org)

# DATA QUALITY METRIC



Records with more specific measurement data are awarded more points than those with less specific data

Scenario 1	Scenario 2	Scenario 2	Scenario 4
Size= 37.5 nm	Size= 37.5 nm	Size= 37.5 nm	Size= 37.5 nm
	Mean Hydrodynamic Diameter	Mean Hydrodynamic Diameter	Mean Hydrodynamic Diameter
		Dynamic Light Scattering	Dynamic Light Scattering
		Malvern ZetaSizer Nano ZS	Malvern ZetaSizer Nano ZS
			11 of 12 measurement parameters reported
			Protocol: ASTM E2490 - 09
<b>Merit</b>	<b>Bronze</b>	<b>Silver</b>	<b>Gold</b>

## Algorithm

Assigns weights to each value in a curated record

$$CL_{PCC} = \sum_{Measurements} \left\{ \frac{\sum_G M_G * P_G}{\sum_G M_G * W_G} \right\}$$



Nanomaterial Registry

**DATA ANALYSIS @ nanoHUB**

# DATA EXPORT



- 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

## DATA EXPORT

**THANK YOU FOR REQUESTING TO EXPORT THE SELECTED DATA!**

Please answer a few demographic questions before you download, so that we are able to better understand the interests of our users. This will not only help us provide a better user interface, but it will also help us in future decisions on what new data to pursue for the Registry.  
Let us know if you have any questions by using the contact form at right.

How would you classify your stakeholder group?\*



Please Select

How would you describe your professional field?\*

Please Select

What are you interested in?\*

Please Select

**EXPORT MY DATA**  

**Additional Information about your download.**  
The Data Export Supplement will help you understand the Registry's data fields (column headings) in the Excel Spreadsheet you download. [You can download The Data Export Supplement here.](#)

# NANOMATERIAL REGISTRY PORTAL



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**

POWERED BY nanoHUB.org

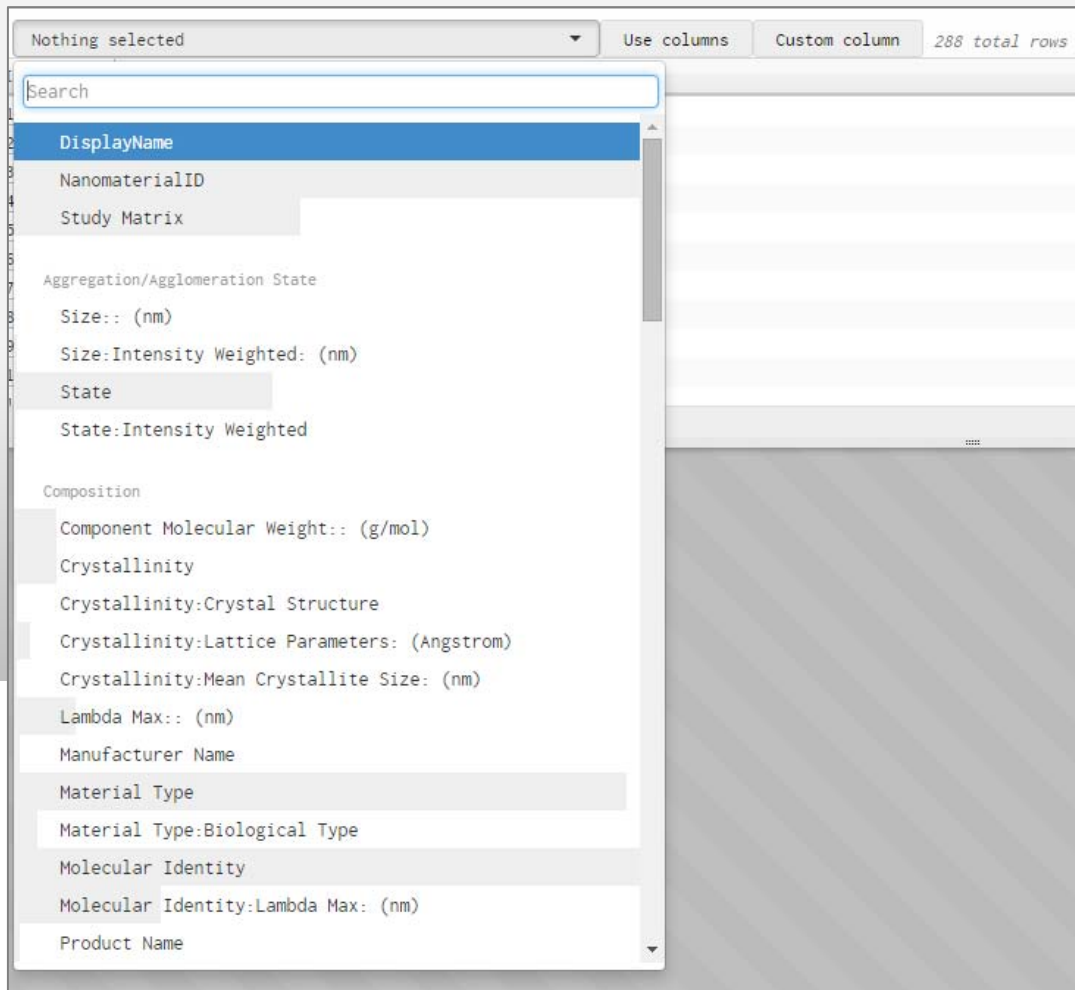
NANOMATERIALREGISTRY

<https://nanohub.org/groups/nanomaterialregistry>

# NANOMATERIAL REGISTRY PORTAL



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 REGISTRY PORTAL



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

Nothing selected ▼ Use columns Custom column 288 total rows Edit filters

ID	DisplayNa...	NanomaterialID	Study Matrix	Mean Hydrodynamic Diameter:: (nm)
1	Ag NP	1		
2	Ag NP	15		
3	Ag NP	35		
4	Ag Np	97		
5	Ag NP	119		
6	Ag	299		
7	Ag NP	338		
8	Ag NP	339		32
9	Ag NP	341		39.6
10	Ag NP	350		47.6
11	Ag NP	351		13.1

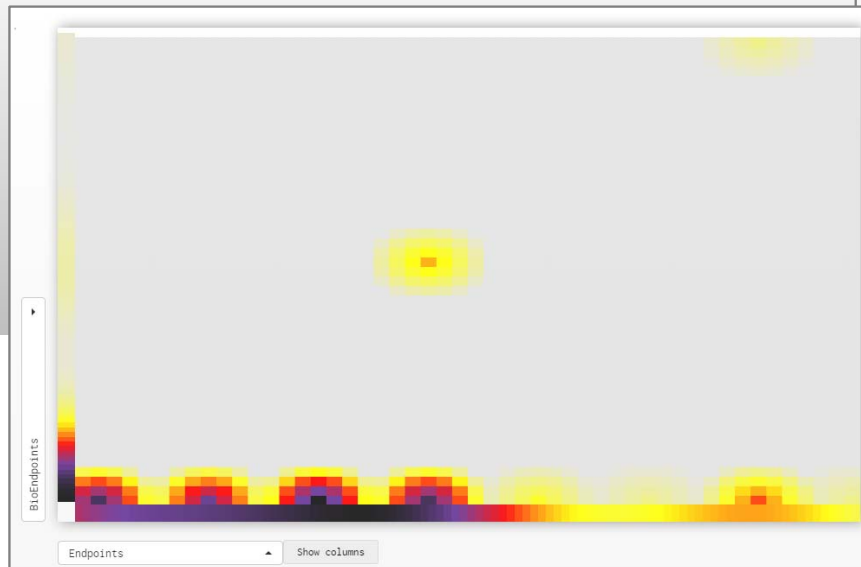
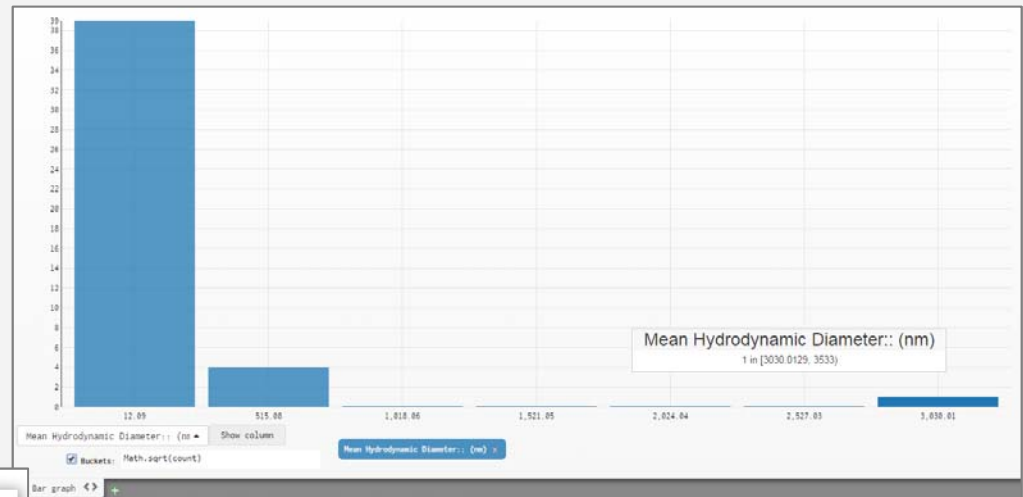
NMRI data +

# NANOMATERIAL REGISTRY PORTAL



Data visualizations available at this time:

- Bar chart
- Heat map



Custom columns can be created with the help of data visualizations

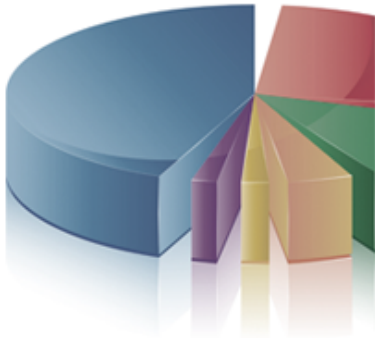
# NANOMATERIAL REGISTRY PORTAL



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

### THE REGISTRY RECORDS

2031 Nanomaterials as of 08/15/2014  
[Visualize Data – Click Here](#)



Search or browse the database using the buttons on this Home page. From a query results table, you can request detailed information on specific nanomaterial records, compare multiple nanomaterials in side-by-side view, and export data to your desktop.

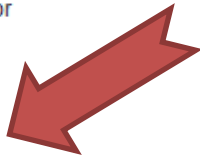
**The Registry provides researchers with a convenient data management and sharing plan.** Both NIH and NSF require grant recipients to have a data management plan. Our curation team is ready to accept your public-ready data, archive them, integrate them with the larger data repository, and share them publicly for you. Visit our [Data Management Plan](#) page to download boilerplate text for your proposal or [contact us](#) for customized text!

**Now available for the predictive modeling community:**  
[The Nanomaterial Registry Portal at nanoHUB](#)

For additional guidance, please refer to our top-menu pages, including the [User Guide](#). To ask questions or provide feedback, please refer to our [Contact Us](#) page.

**December 2014** - Nature will begin a new author checklist in January 2015 focused on data reproducibility through thorough data sharing during publication ... [Read more](#)

[SEE ALL NEWS ▶](#)

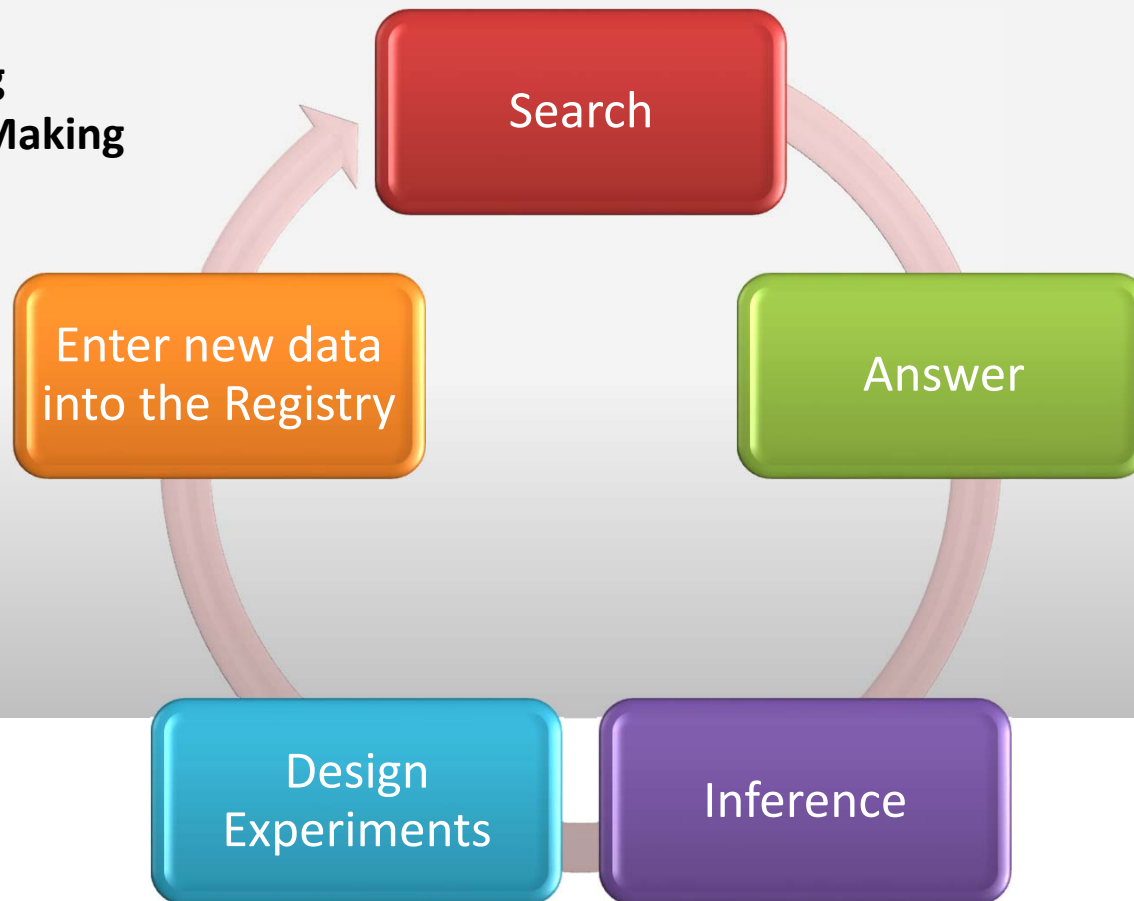


[www.nanomaterialregistry.org](http://www.nanomaterialregistry.org)

# STATE OF THE SCIENCE

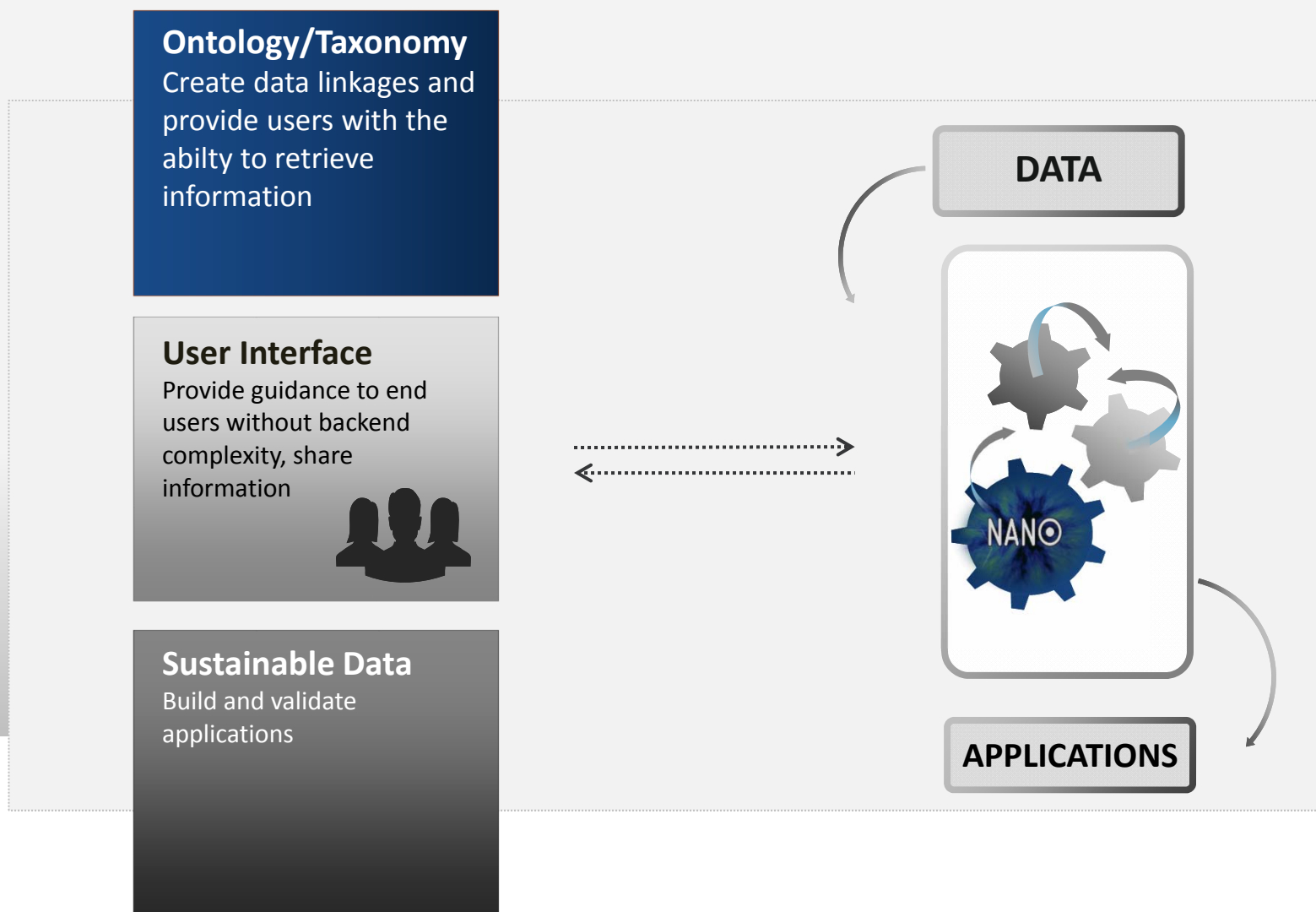
## Evolving Registry and Tools

- Gap Filling
- Decision Making

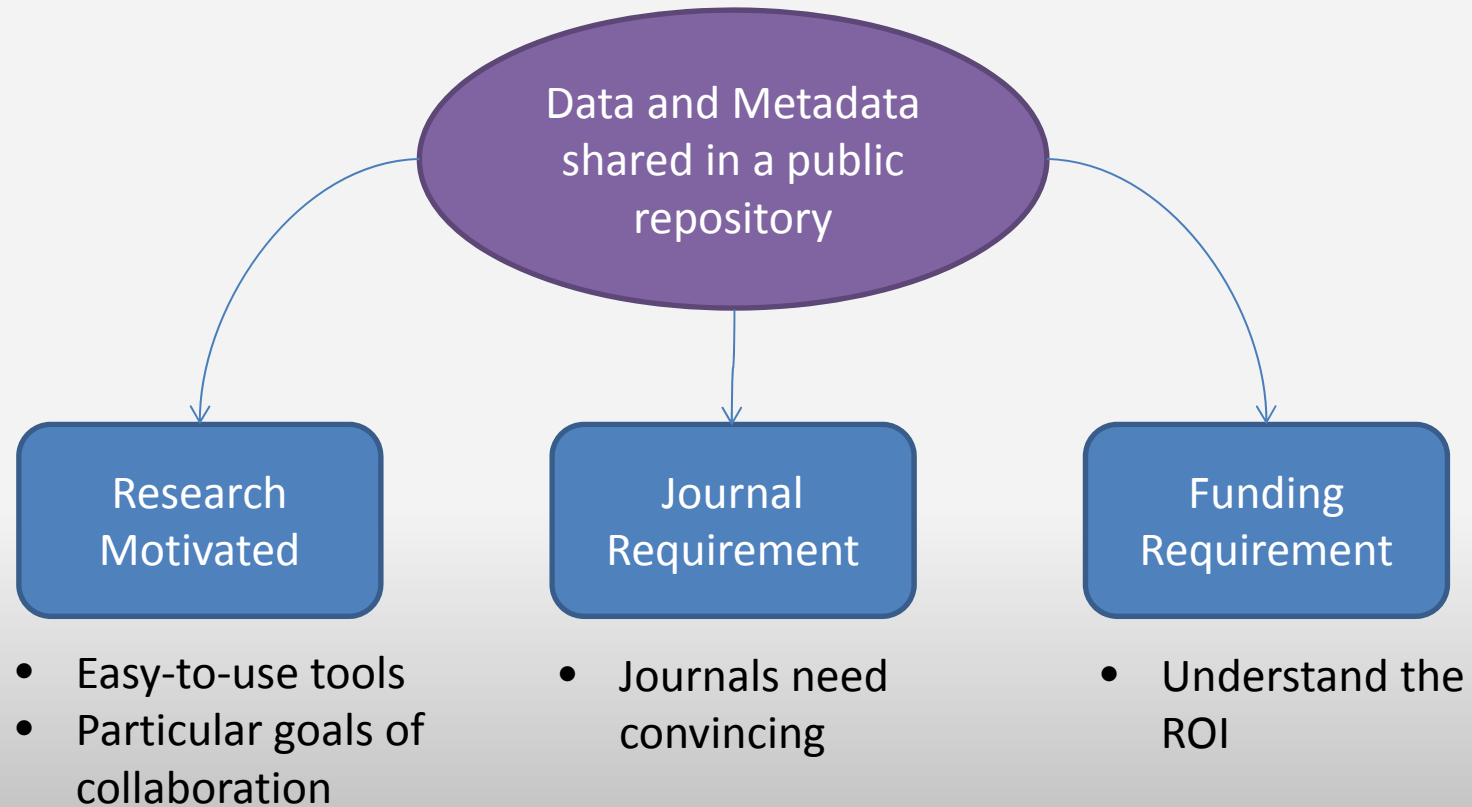




# LINKING AND SHARING INFORMATION



# DATA SHARING





The screenshot shows the top portion of a web page for Nature Nanotechnology. The header is orange with the journal title in white. Below the header is a navigation bar with links for Home, Current issue, Comment, Research, Archive, Authors & referees, and About the journal. A breadcrumb trail reads: home > current issue > editorial > full text. The article title is "Joining the reproducibility initiative" and the journal name is "NATURE NANOTECHNOLOGY | EDITORIAL". The article details are: "Nature Nanotechnology 9, 949 (2014) | doi:10.1038/nnano.2014.287" and "Published online 03 December 2014". There are icons for sharing, email, and printing on the right side.

“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.

# NANOMATERIALREGISTRY

Thank You!

[www.nanomaterialregistry.org](http://www.nanomaterialregistry.org)

[nanoregistry@rti.org](mailto:nanoregistry@rti.org)

## Select Project Publications

- Ostraat, M., Mills, K. C., Murry, D. A., Guzan, K. A. (2012). Nanomaterial Registry: Opportunities and Challenges in Informatics. *In 2012 IEEE International Conference on Bioinformatics and Biomedicine Workshops*, pp. 884–888.
- Ostraat, M., Mills, K. C., Guzan, K. A., & Murry, D. A. (2013). The Nanomaterial Registry: Facilitating the Sharing and Analysis of Data in the Diverse Nanomaterial Community. *International Journal of Nanomedicine*, 8(Suppl 1), 7–13. doi:10.2147/IJN.S40722
- Guzan, K. A., Mills, K. C., Gupta, V., Murry, D. A., Scheirer, C. N., Willis, D. A., & Ostraat, M. (2013). Integration of data: The Nanomaterial Registry project and data curation. *Computational Science and Discovery*, 6(1), 1–8.
- Mills, K. C., Murry, D. A., Guzan, K. A., & Ostraat, M. (2014). Nanomaterial Registry: database that captures the minimal information about nanomaterial physico-chemical characteristics. *Journal of Nanoparticle Research*, 16, 2219. doi:10.1007/s11051-013-2219-8
- Guzan, K. A., Gupta, V., Mills, K. C., & Ostraat, M. (2014). A Nanomaterial Registry. In Matthew Hull and Diana Bowman (Eds.), *Nanotechnology Environmental Health and Safety, Second Edition: Risks, Regulation, and Management*. (pp. 153–172). Waltham, MA: Elsevier.