



Nanotechnology databases and ontology: US resources

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Objectives of the CoR

- Identification of the data elements necessary to establish common data-sharing model(s)
- Specification of requirements for sharing data between research groups and repositories in human- and machine-interpretable forms
- Definition of concepts necessary to support the above activities and representation of those concepts in an ontological framework



Goals for this presentation

- Provide overview of select available resources from US
- Stimulate discussion about
 - Common data elements
 - Common terminology needs
 - Priorities for data sharing and search



Data resources

caNanoLab

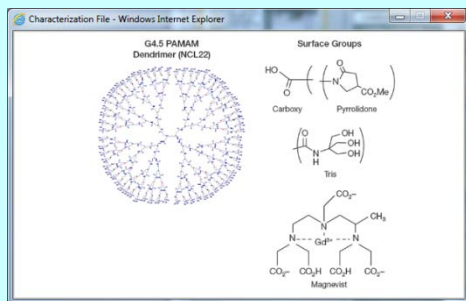
<https://cananolab.nci.nih.gov>

- caNanoLab is a portal designed to facilitate data sharing in the research community to expedite and validate the use of nanomaterials in biomedicine
- caNanoLab provides support for the annotation of nanomaterials with composition information, characterizations, and protocols
- caNanoLab leverages and extends concepts from the NCI's Enterprise Vocabulary Services (EVS) and the NanoParticle Ontology (NPO)

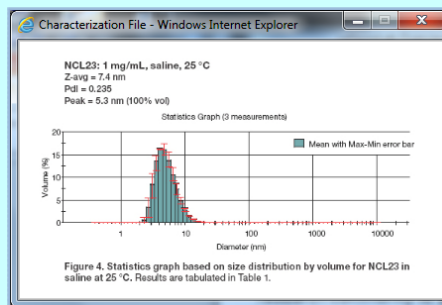
The screenshot shows the caNanoLab website in a web browser. The header includes the National Cancer Institute logo and the text "caNanoLab". The main content area features a "Welcome to caNanoLab" message and a table with search results. The table has two columns: "Data Type" and "Public Results".

Data Type	Public Results
Search Protocols Search for nanotechnology protocols leveraged in performing nanomaterial characterization assays.	37
Search Samples Search for information on nanomaterials including the composition of the nanomaterial, results of physico-chemical, in vitro, and other characterizations, and associated publications. See also Advanced Sample Search .	957 62 Sample Sources 3588 Characterizations 1216 Physico-chemical 1925 In Vitro 448 Other
Search Publications Search for information on nanotechnology publications including peer reviewed articles, reviews, and other types of reports related to the use of nanotechnology in biomedicine.	1079

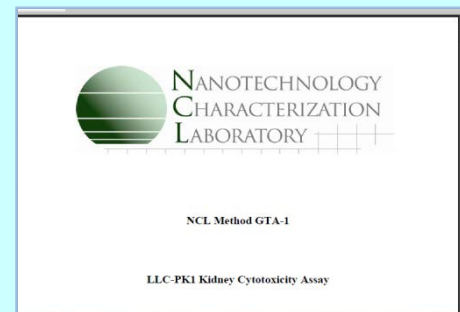
Below the table, it says "Last updated on 2012-10-10 13:00:27". To the right of the table, there is a "Features" section listing various capabilities of the portal, such as "Secure submission of protocols, samples (nanomaterials), and publications" and "Basic search facilities for searching for protocols, samples, and publications". There is also a "How To" section with frequently asked questions.



Composition



Characterizations



Protocols

A tool for the storing, sharing, and analysis of data from the nanomaterial community

WELCOME TO THE NANOMATERIAL REGISTRY!

The Nanomaterial Registry is a one-stop, authoritative, fully curated resource that provides information on the biological and environmental implications of well-characterized nanomaterials.

The Nanomaterial Registry is being built through strong collaborations with broad stakeholder groups that represent the diverse nanomaterial community, including industry, regulatory institutions, government, and academia. [LEARN MORE ABOUT OUR VISION](#) [WHAT IS CURATED DATA?](#)

Nanomaterial Registry

Minimal Information Standards

Compliance Levels

Instance of Characterization

Matching & Similarity

Comparison

BROWSE NANOMATERIALS



Material Type



Size



Shape



Surface Area

A TOOL FOR THE NANOMATERIAL COMMUNITY

An authoritative website that compiles data from multiple databases into a single resource, the Nanomaterial Registry (NR) provides tools for analyzing and comparing data on the biological and environmental implications of well-characterized nanomaterials. This resource will evolve as the quality and quantity of the information on nanomaterials improve. Hundreds of nanomaterial entries have been curated into the NR for physico-chemical characteristics and are available to the public. Biological and environmental study data for existing nanomaterial entries will also be curated into the NR.

To access this information, search or browse the database using the buttons on this home page. From a query results table, you can request portions of the data. From a query results table, you can request to access the information, search or browse the database using the

study data for existing nanomaterial entries will also be curated into the NR. The NR provides a one-stop, authoritative, fully curated resource that provides information on the biological and environmental implications of well-characterized nanomaterials. This resource will evolve as the quality and quantity of the information on nanomaterials improve. Hundreds of nanomaterial entries have been curated into the NR for physico-chemical characteristics and are available to the public. Biological and environmental study data for existing nanomaterial entries will also be curated into the NR.

LATEST NEWS

June 2012 - The Greener Nano 2012: Nanoinformatics Tools and Resources Workshop, will be held in Portland, OR, July 30th... [Read more](#)

May 2012 - The U.S. Government Accountability Office has released a report, "Nanomaterials: The U.S. Office has released a report on government accountability May 2012 - The U.S.

Funded by:



NIEHS

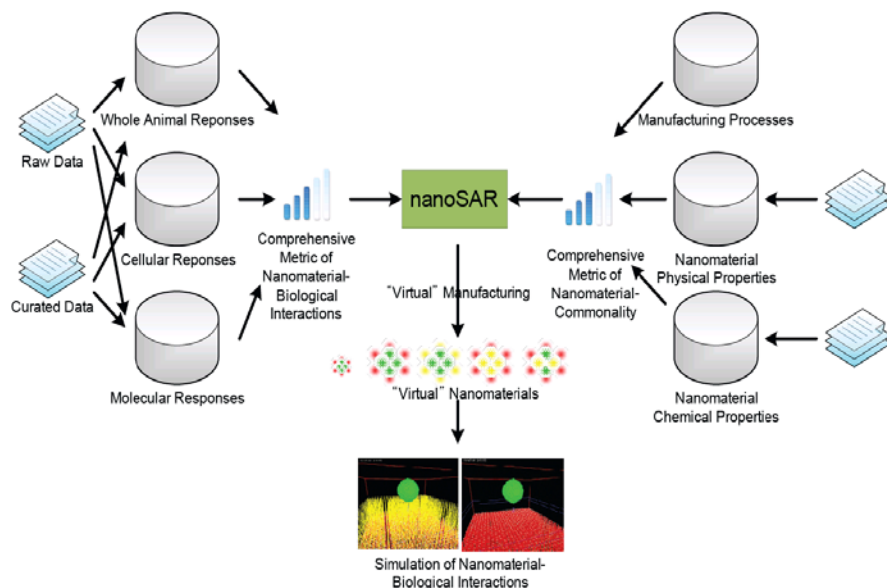
NIBIB

NATIONAL
CANCER
INSTITUTE

RTI
INTERNATIONAL

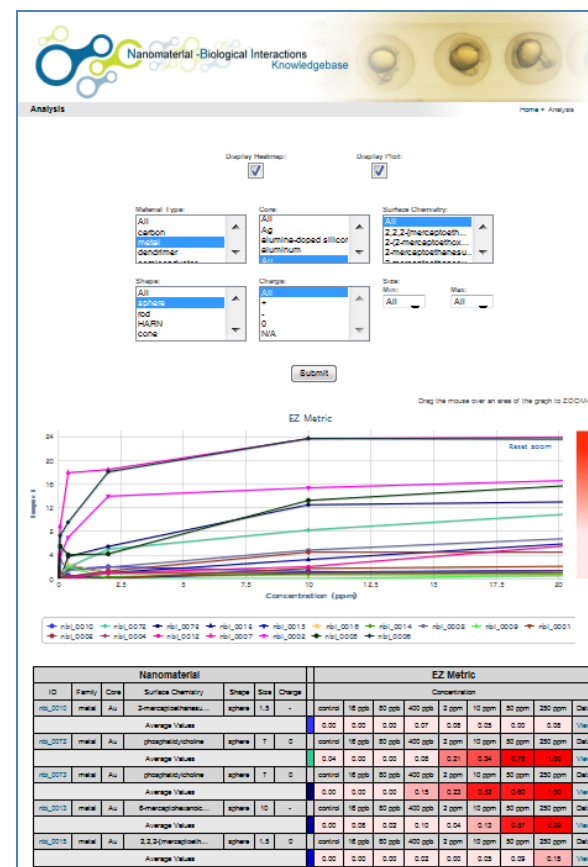
Goals and Objectives

- To serve as a repository for annotated data on the physicochemical properties of nanomaterials and their biological interactions
- To organize and analyze data and compare results across research platforms in an effort to define robust structure-activity relationships
- To identify the functional design principles of high performing, environmentally-benign nanomaterials
- To predict potential biological impacts of unsynthesized nanomaterials



Features

- Easy to use tab-formatted downloadable spreadsheets for material and experimental records
- Alignment with ISA-TAB-Nano allows data exchange with other groups
- Built in heat mapping and graphical data representation

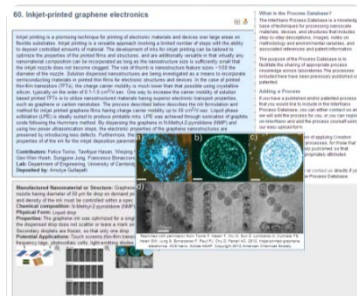
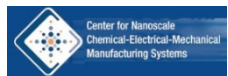


To support and help launch communities of practice in nanomanufacturing in both real and cyber space

A catalyst for nanomanufacturing R & D advancement in the US via:

- Cooperative activities (workshops, conference, initiatives)
- An information clearinghouse (InterNano)
- Nanoinformatics leadership
- Thematic workshops
- Education and training
- ISO TC 229 standards project *Terminology and Definitions for Nanomanufacturing Processes*

key partners & affiliates



Process database techniques for processing nanoscale materials, devices, and structures



Nanomanufacturing taxonomy



More features:

- Expert reviews
- Columns
- Directory
- Research library
- News
- Newsletters

Mark Tuominen - NNN Director * Jeff Morse - NNN Managing Director

Jessica Adamick – InterNano Project Manager * Robert Stevens – Web Development



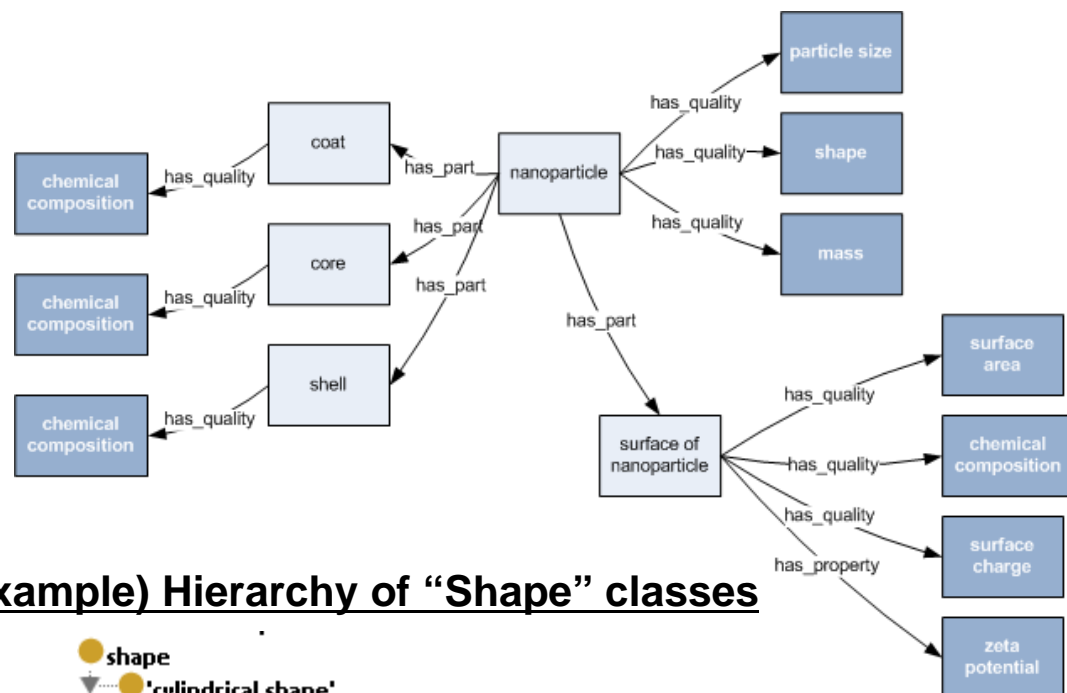


Ontology and data-sharing formats

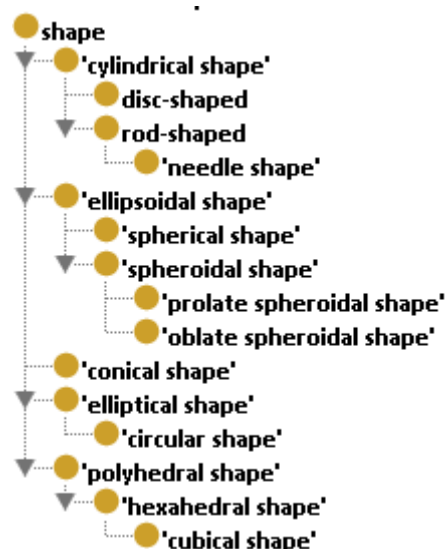
NanoParticle Ontology (NPO)



- Ontology for representing knowledge underlying the description, preparation, and characterization of nanomaterials
- Includes terms from other biomedical ontologies
- Provides logical relations between terms
- Purpose
 - Common vocabulary
 - Data annotation
 - Semantic integration of data
 - Unambiguous interpretation of data
 - Knowledge-based searching
 - Knowledge-framework for developing data sharing models and standards



(Example) Hierarchy of “Shape” classes



Reference:

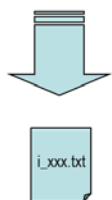
D. G. Thomas, R. V. Pappu and N. A. Baker, NanoParticle Ontology for cancer nanotechnology research, *Journal of Biomedical Informatics* 44 : 59-74 (2011).

ISA-TAB-Nano



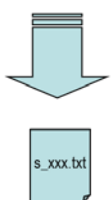
- A standard tab-delimited format for describing nanotechnology data
- Leverages and extends the Investigation/Study/Assay (ISA-TAB) format
 - Standard tab-delimited file format
 - Developed by the European Bioinformatics Institute (EBI) for representing a variety of assays and technology types
- **ISA-TAB-Nano supports ontology-based curation**
 - Nanomaterials and concepts from the NanoParticle Ontology (NPO) as well as other ontologies

1. Describe the Investigation and Studies

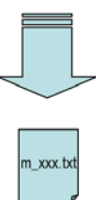


Investigation File

2. Identify Study Samples

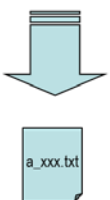


Study File(s)



Material File(s)

3. Record Assay Conditions and Measurements



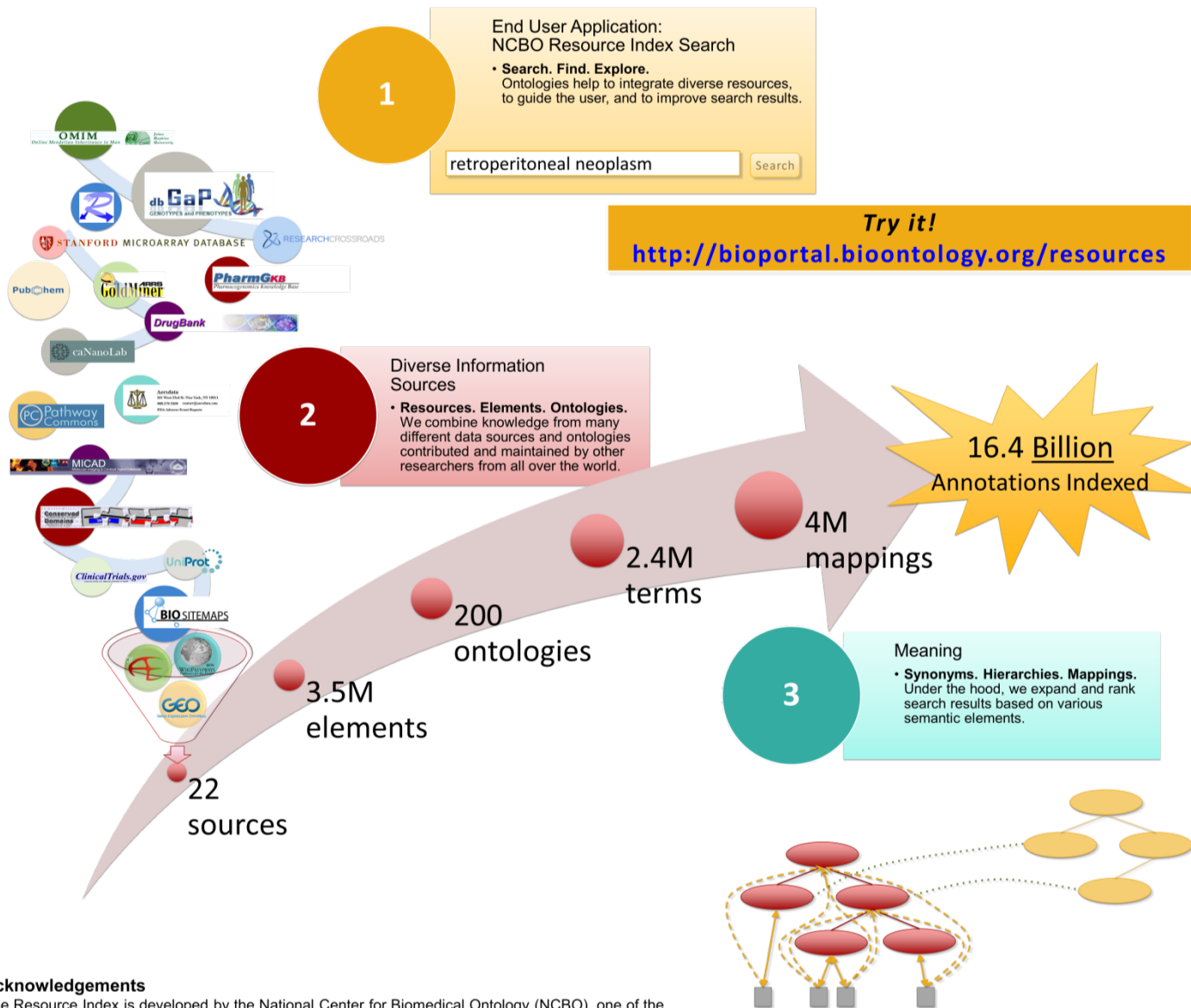
Assay File(s)

Ontology References

ONTOLOGY SOURCE REFERENCE		
Term Source Name	MO	NPO
Term Source File	http://purl.bioontology.org/ontology/MO	http://purl.bioontology.org/ontology/npo
Term Source Version	v. 1.3.1.1	v. 2011-02-12
Term Source Description	MGED Ontology	NanoParticle Ontology
INVESTIGATION		
Investigation Identifier	NCL200612A	
Investigation Title	Dendrimer-Based MRI Contrast Agents	
Investigation Description	The goal of this investigation is to characterize a PAMAM dendrimer with an	
Investigation Disease		
Investigation Disease Term Accession Number		
Investigation Disease Term Source REF		
Investigation Outcome		
Investigation Submission Date	2002-11-30	
Investigation Public Release Date	2002-11-30	
INVESTIGATION CONTACTS		
Investigation Person Last Name	McNeil	
Investigation Person First Name	Scott	
Investigation Person Middle Initials	E	
Investigation Person Email	mcneils@mail.nih.gov	
Investigation Person Phone	3018466939	
Investigation Person Fax		
Investigation Person Address	MSC 1050 Boyles Street, Frederick, MD 21702	
Investigation Person Affiliation	Nanotechnology Characterization Laboratory	
Investigation Person Role	Investigator	
Investigation Person Role Term Accession Number		
Investigation Person Role Term Source REF	MO	
INVESTIGATION PUBLICATIONS		
Investigation PubMed ID	18095846	
Investigation Publication DOI	10.2217/17435889.2.6.789	
Investigation Publication Author List	Hall JB; Dobrovolskaia MA; Patri AK; McNeil SE	
Investigation Publication Title	Characterization of nanoparticles for therapeutics	
Investigation Publication Status	published	
Investigation Publication Status Term Accession Number		
Investigation Publication Status Term Source REF		

Investigation Contacts

Investigation Publications





Summary

- Several different points for collaboration and interaction
- Resources
 - caNanoLab (<https://cananolab.nci.nih.gov/caNanoLab/>)
 - NBI (<http://nbi.oregonstate.edu/>)
 - Nanomaterial Registry
(<https://www.nanomaterialregistry.org/>)
 - InterNano (<http://www.internano.org/>)
- Ontology and data-sharing
 - NanoParticle Ontology (<http://www.nano-ontology.org/>)
 - ISA-TAB-Nano (<https://wiki.nci.nih.gov/display/ICR/ISA-TAB-Nano>)
 - NCBO Bioportal (<http://bioportal.bioontology.org/>)