A Joint Workshop 2012

eu-us bridging nanoEHS research efforts

25-26 OCTOBER 2012, HELSINKI, FINLAND

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

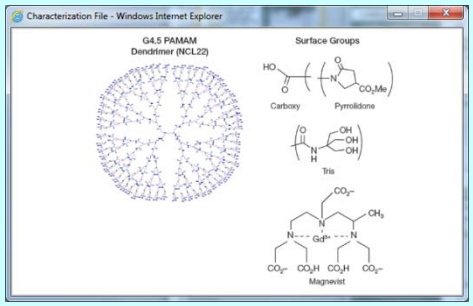
- Provide overview of *select* available resources from US
- Stimulate discussion about
  - Common data elements
  - Common terminology needs
  - Priorities for data sharing and search

Data resources

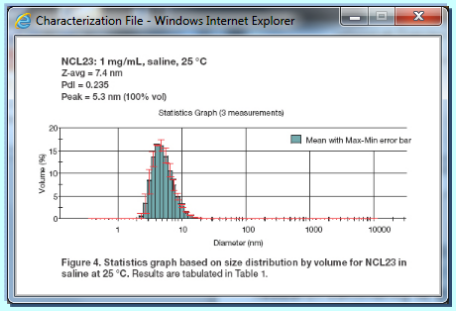
caNanoLab

https://cananolab.nci.nih.gov

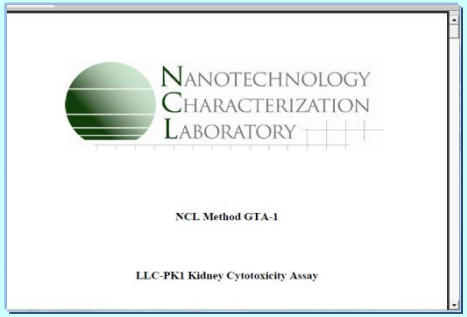
- caNanoLab is a portal designed to facilitate data sharing in the research community to expedite and validate the use of nanomaterials in biomedicine
- caNanoLab provides support for the annotation of nanomaterials with composition information, characterizations, and protocols
- caNanoLab leverages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



Composition



Characterizations

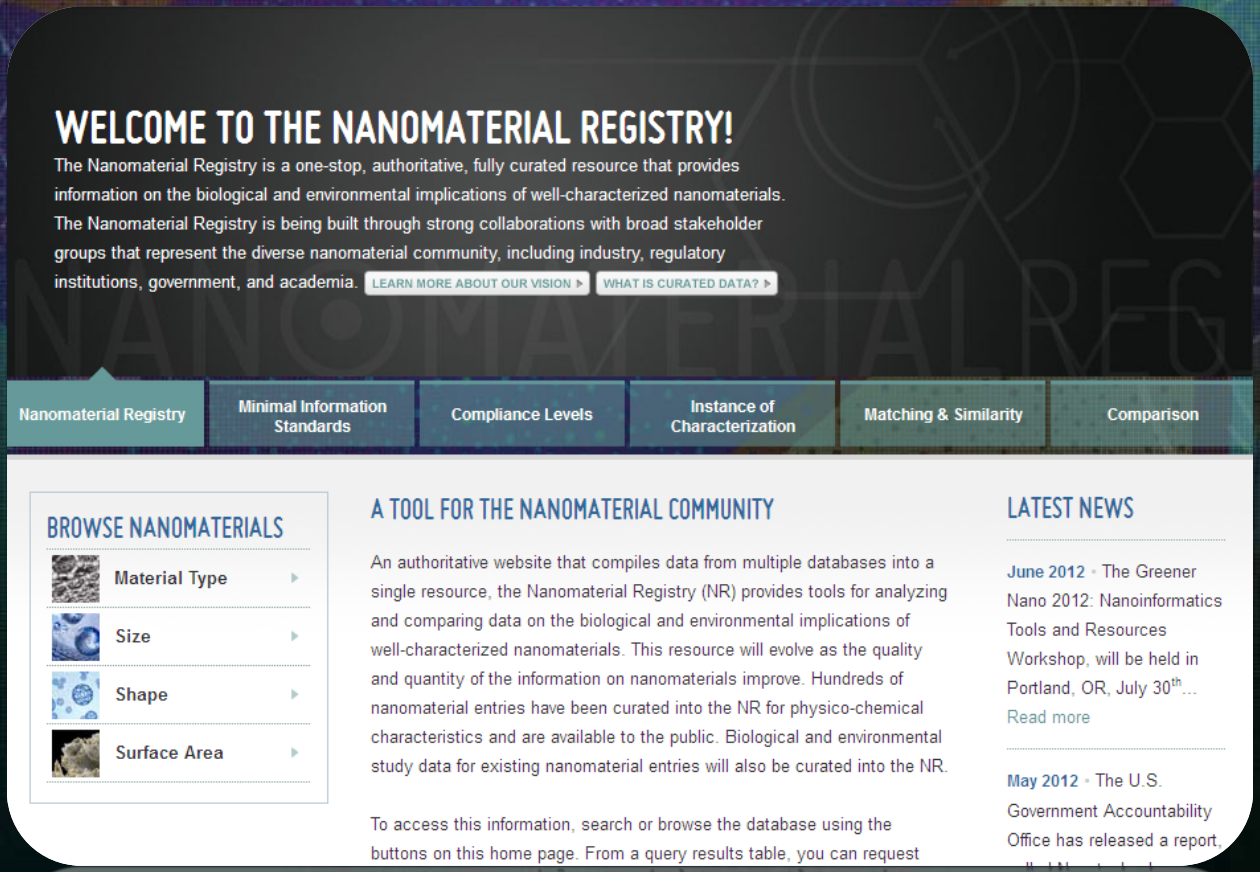


Protocols

NANOMATERIALREGISTRY

Web Address:
www.nanomaterialregistry.org

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



Funded by:

NIEHS

NIBIB

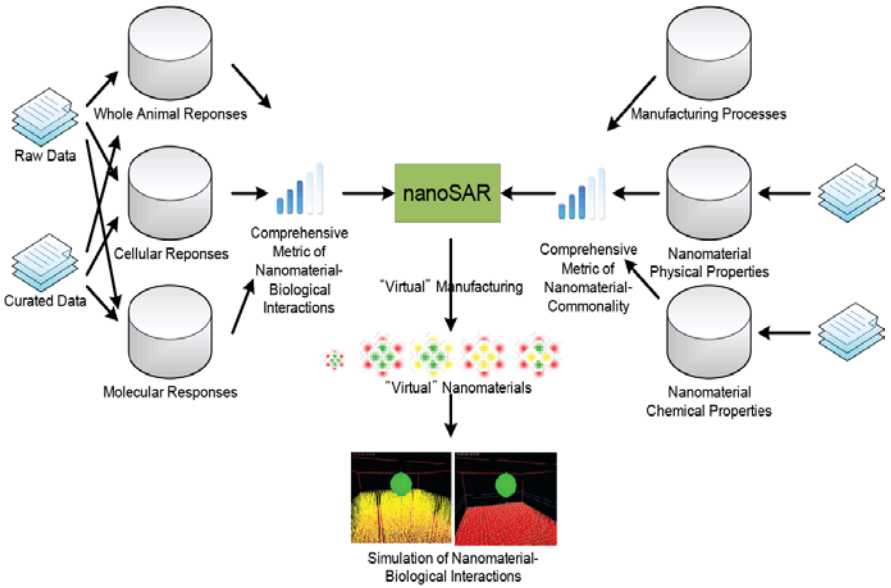
National Cancer Institute

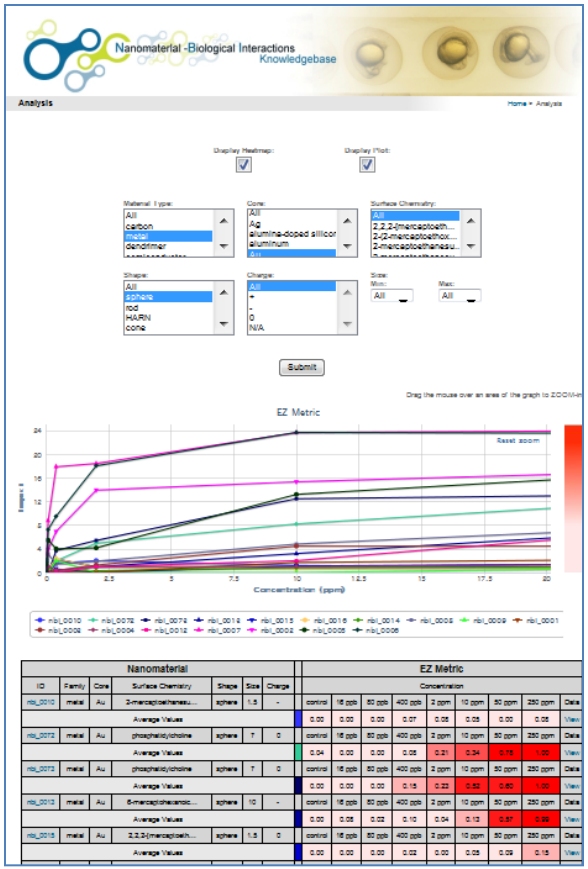
RTI International

Nanomaterial -Biological Interactions Knowledgebase

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

http://nbi.oregonstate.edu

National Nanomanufacturing Network

InterNano

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

CHM Center for Hierarchical Manufacturing University of Massachusetts Amherst

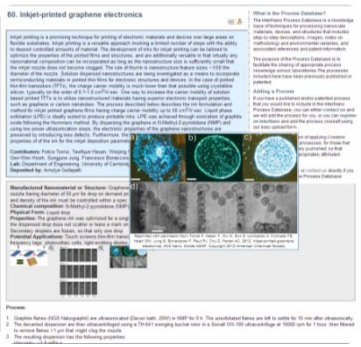
Center for High-rate Nanomanufacturing

SINAM CENTER FOR SCALABLE AND INTEGRATED NANOMANUFACTURING

Center for Nanoscale Chemical-Electrical-Mechanical Manufacturing Systems

CNST

NanoBusiness COMMERCIALIZATION ASSOCIATION



Process database

techniques for processing nanoscale materials, devices, and structures

Nanomanufacturing taxonomy

More features:

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

CHM Center for Hierarchical Manufacturing University of Massachusetts Amherst

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

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

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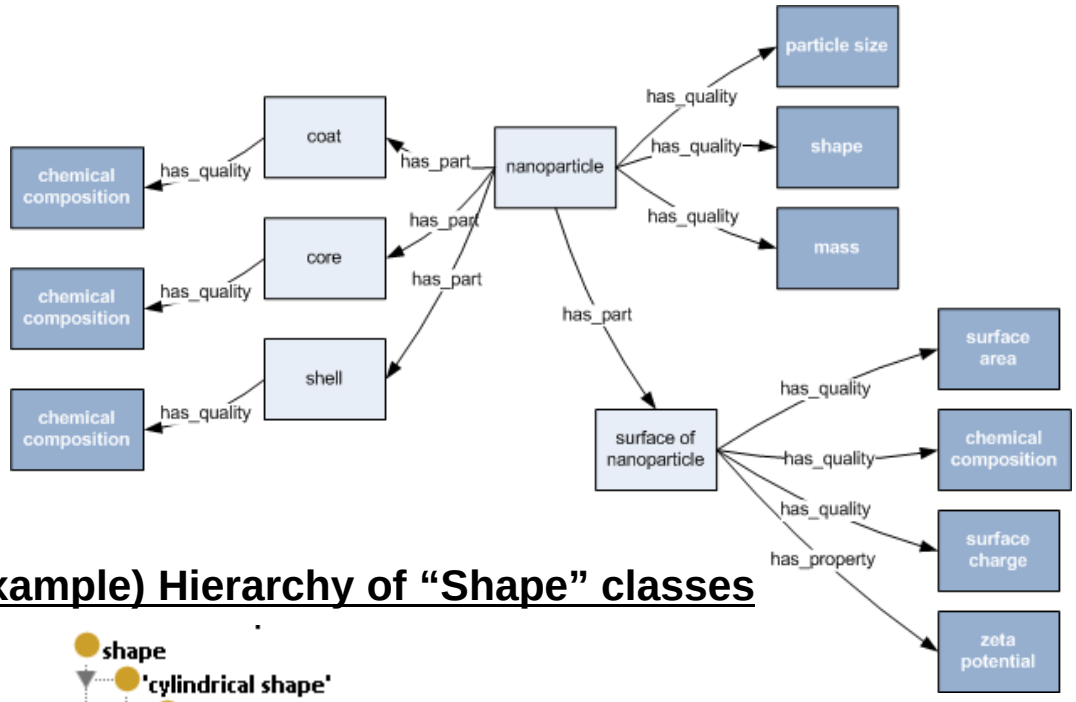
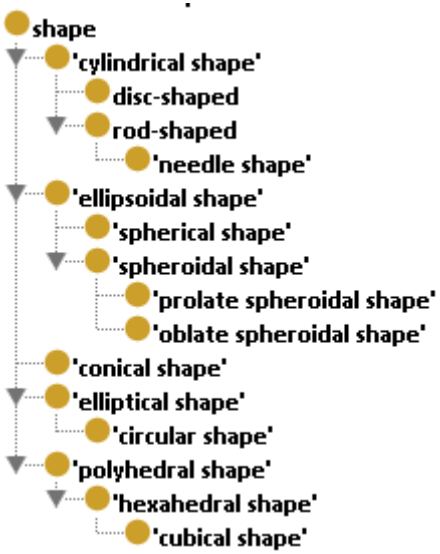
Ontology and data-sharing formats

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

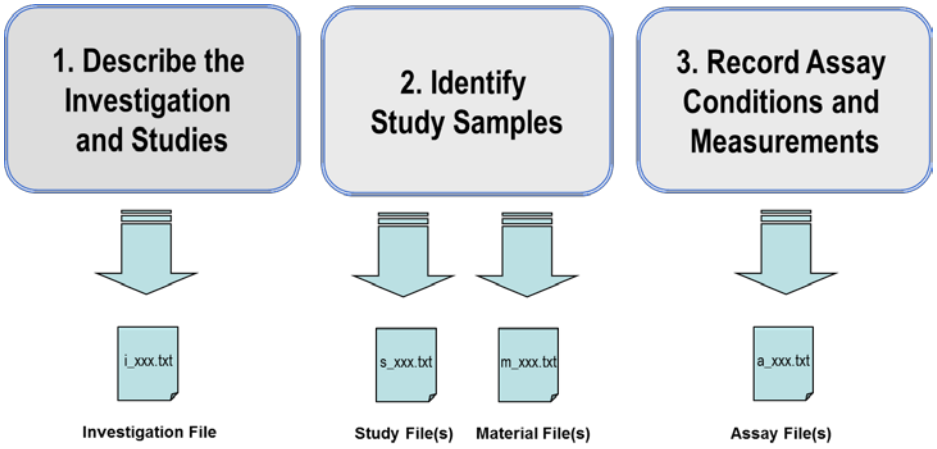


Reference:
D. G. Thomas, R. V. Pappu and N. A. Baker, NanoParticle Ontology for cancer nanotechnology research, *Journal of Biomedical Informatics* 44 : 59-74 (2011).

caBIG cancer Biomedical Informatics Grid™

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



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 Description	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 Contacts	Investigation Person Last Name	McNeil	
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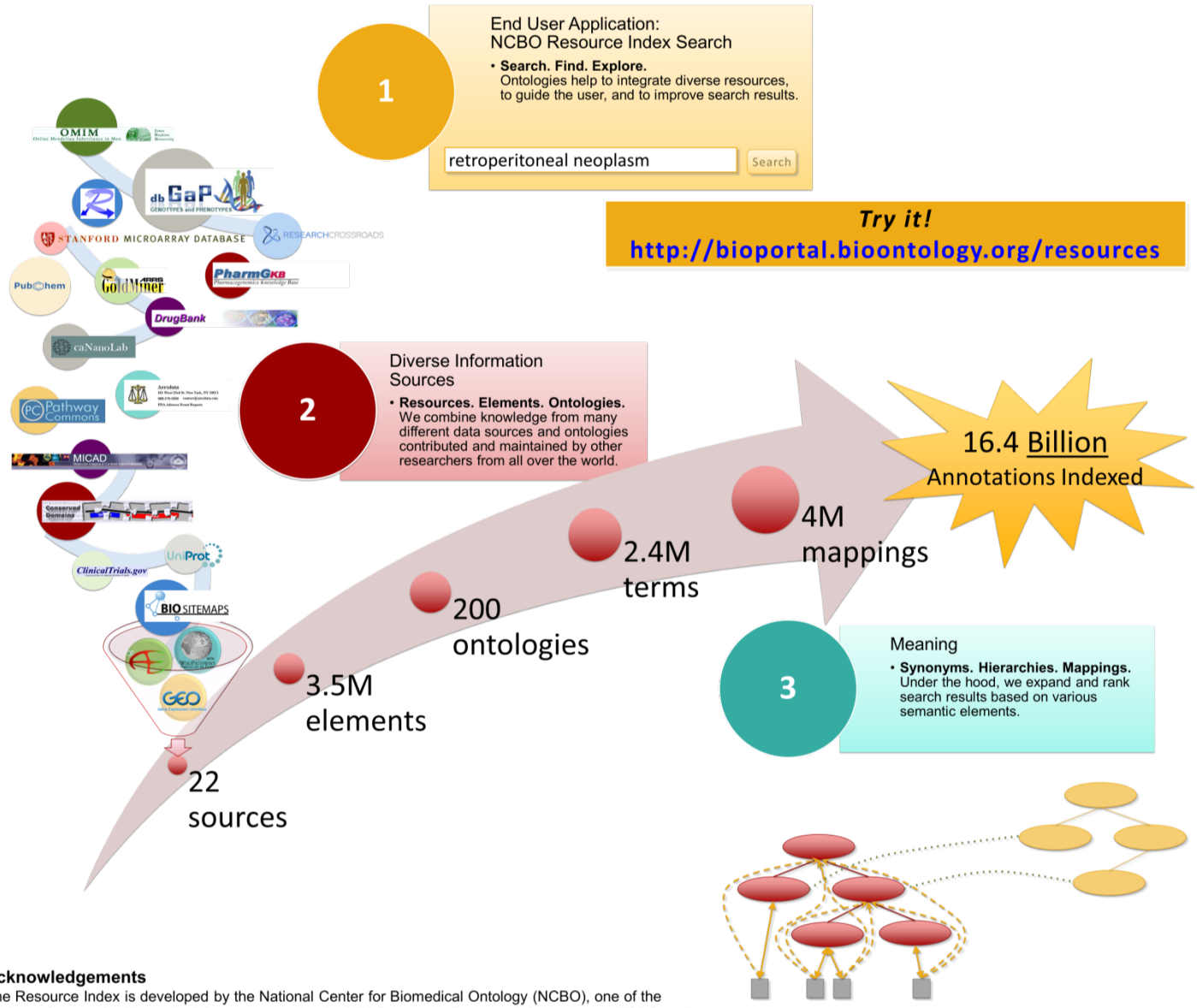
	Investigation Person Address	MSC 1050 Boyles Street, Frederick, MD 21702	
	Investigation Person Affiliation	Nanotechnology Characterization Laboratory	
	Investigation Person Role	investigator	
	Investigation Person Role Term Accession Number		
	Investigation Person Role Term Source REF	MO	
	INVESTIGATION PUBLICATIONS		
Investigation 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		

THE NATIONAL CENTER FOR BIOMEDICAL ONTOLOGY

NCBO Bioportal



Acknowledgements

The Resource Index is developed by the National Center for Biomedical Ontology (NCBO), one of the National Centers for Biomedical Computing under the NIH Roadmap. For more information on NCBO and working with the Center, visit http://www.bioontology.org or email support@bioontology.org.

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/)