Informatics and standards for nanomedicine technology

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Outline

- **Introduction to the caBIG® Nanotechnology Working Group**
- Overview of nanotechnology informatics challenges
- Research projects
  - Ontology development
  - PubNano resource
  - Data exchange standards
  - Structure-property-activity modeling

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National Cancer Institute caBIG® Nanotechnology Working Group

- Government
  - National Institutes of Health
    - NCI, NHLBI, NIBIB, NCL
  - Center for Disease Control
  - Food and Drug Administration
  - Environmental Protection Agency
  - …
- Academia
  - Washington University
  - Pacific Northwest National Lab
  - Oregon State
  - Stanford
  - MIT
  - Georgia Tech
  - UCLA
  - …
- Industry
  - Intel
  - Pennsylvania NanoSystem
  - …
- Standards organizations
  - ASTM E56
  - ISO TC229
- Alliances and organizations
  - International Alliance for NanoEHS Harmonization
  - Oregon Nanoscience and Microtechnologies Institute
  - National Nanotechnology Initiative
  - National Nanomanufacturing Network
  - NCI Nano Alliance

caBIG™ cancer Biomedical Informatics Grid ™

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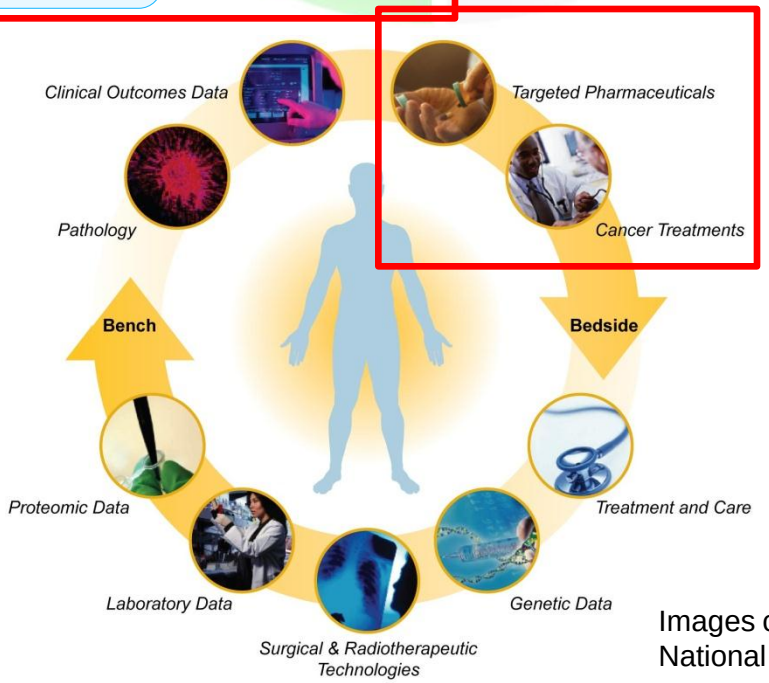
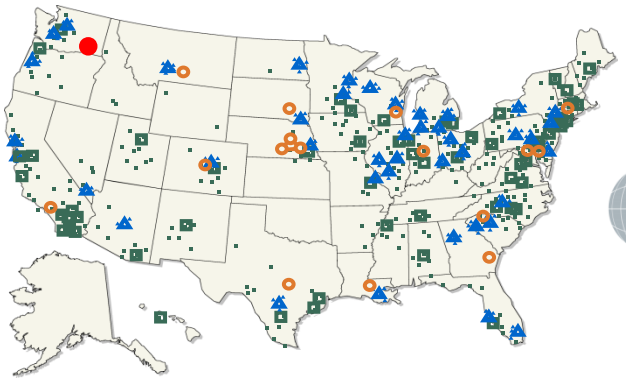
caBIG® Overview (http://cabig.nci.nih.gov/)



- Bench-to-bedside biomedical research infrastructure
- Integrates basic research to clinical research to patient care
- Broad deployment
  - Extensible framework
  - Significant use outside the cancer domain
- Poised for significant growth



caBIG™ cancer Biomedical Informatics Grid™

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Images courtesy of Juli Klemm, National Cancer Institute

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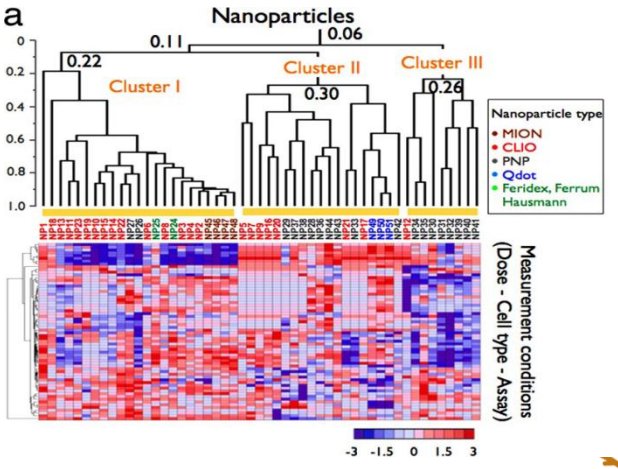
Working Group Scope



Shaw et al., 2008. *PNAS*, 105: 7387.

Sharon Gaheen, SAIC

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Nano WG current areas of focus

- Nano-TAB development (*enabling*)
  - Nanotechnology data sharing standards
  - Working draft ready
  - Community engaged
  - Need to focus on applications and standards
- NPO support and expansion (*enabling*)
  - Standard vocabulary and ontology for nanomedicine
  - Foundation established
  - Community engaged
  - Need to focus on support for nano-TAB and other annotation projects
- Nano-QSAR (*applying*)
  - Structure-activity relationships for nanomaterial-biological interactions
  - Community engaged; participants identified
  - Many potential areas of focus

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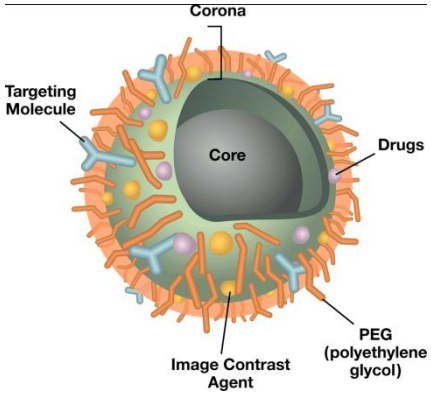
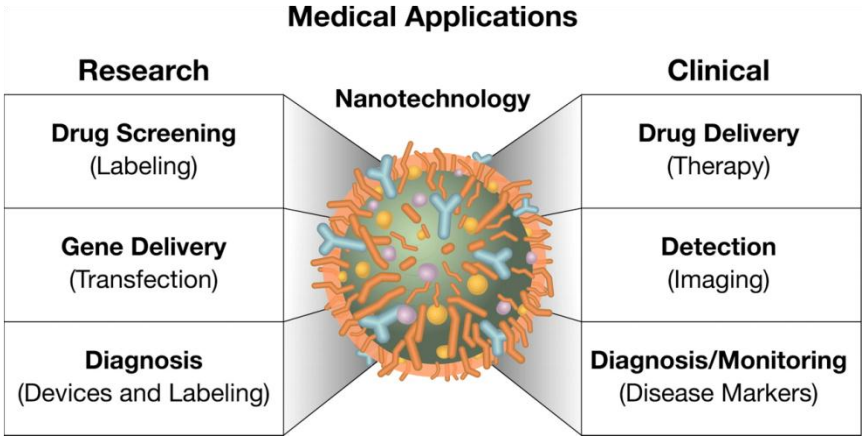
What is the problem? *Unrealized potential due to combinatorial complexity*

- Nanomaterials are small and diverse
- The promise:
  - High density
  - Improved biodistribution
  - Multi-modal applications
- The problems:
  - Combinatorial diversity
  - Difficult characterization
- ***An important challenge!***





McNeil SE. *J Leukoc Biol*, 2005. **78**(3): p. 585-94. doi:10.1189/jlb.0205074

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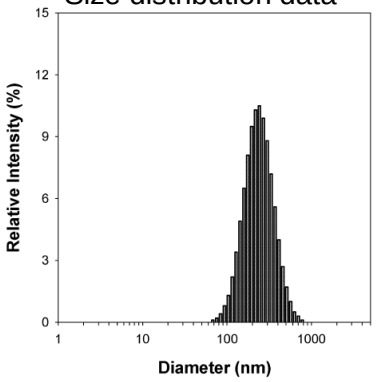
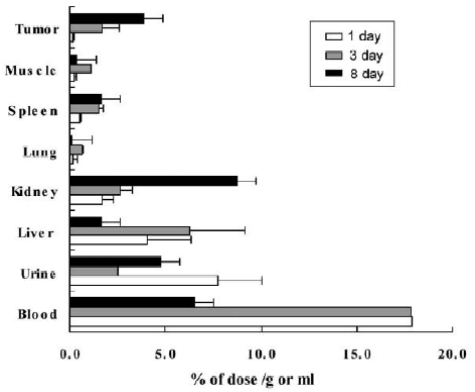
What is the problem? *Diversity of data*

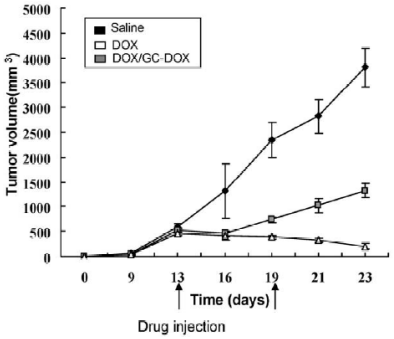
Size distribution data

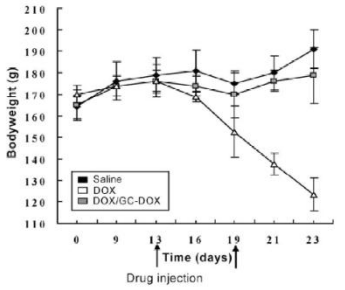


Tissue biodistribution

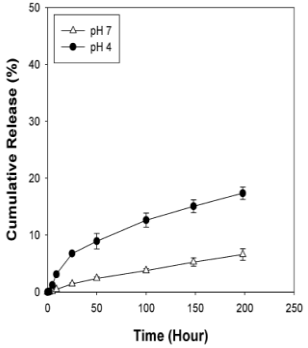


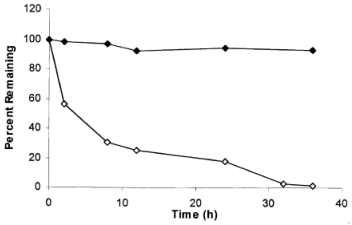
Anti-tumor activity

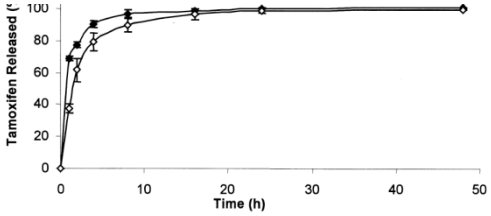




In vitro drug release







Zeta Potential

Table 1
Zeta potential values of control and tamoxifen loaded nanoparticles[a]

Nanoparticle formulations	Zeta potential (mV)
Control nanoparticles	6.7±1.2[b]
Tamoxifen-loaded nanoparticles	25.4±1.4

[a] Zeta potentials of the nanoparticle suspension in deionized distilled water were measured using the Brookhaven's Zeta PALS instrument.
[b] Mean ±S.D ($n = 8$).

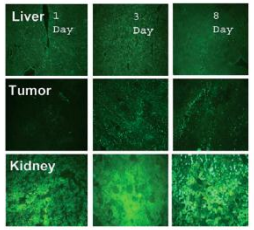
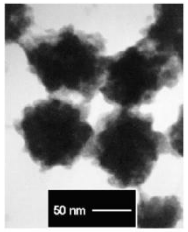
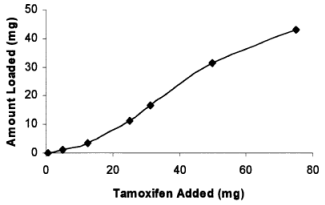


Fig. 8. Tissue accumulation of FITC-conjugated glycol-chitosan (FTC-GC) nanoaggregates for 8 days after i.v. injection in tumor-bearing rats at a dose of 10 mg/kg. Tissue accumulation measured by fluorescence microscopy.

Surface morphology data

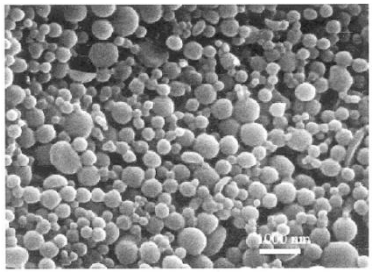


Drug loading data



Preparation

Chemical composition of nanoparticle formulation



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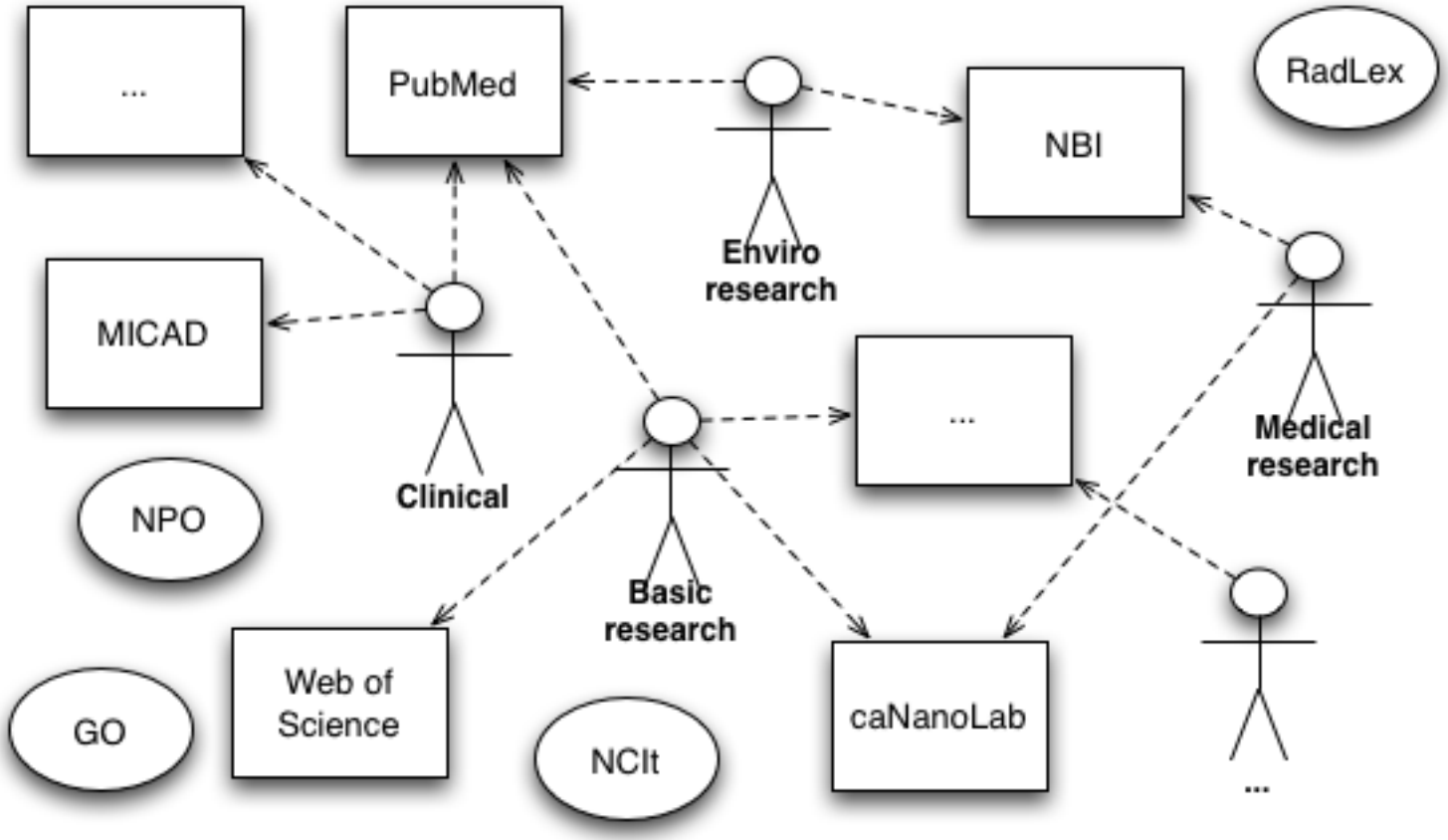
Source: Chawla JS et al, *Int J Pharm*, **249**, 127-38 (2002), Son YJ et al, *J Control Release*, **91**, 135-145 (2003)

What is the problem? *Disconnected resources and users*



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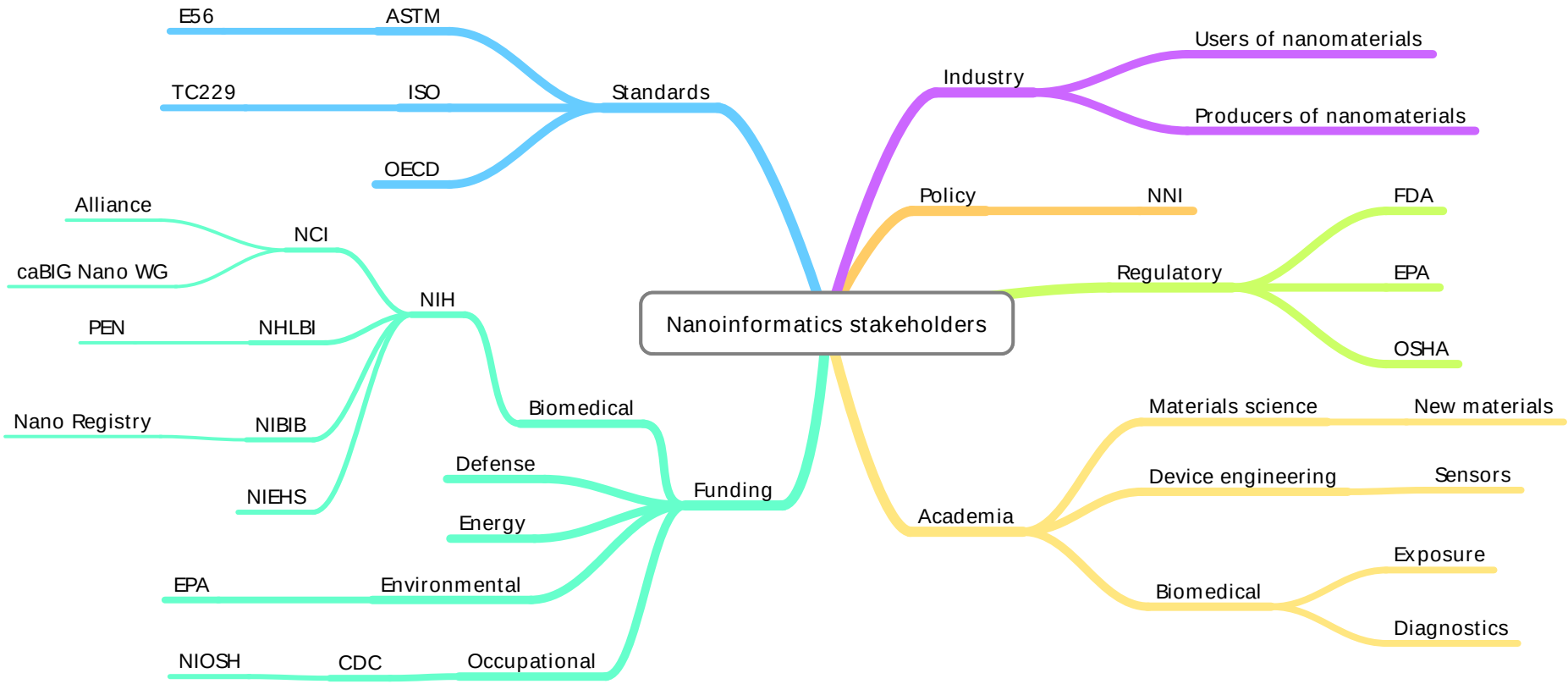
Who are the stakeholders?



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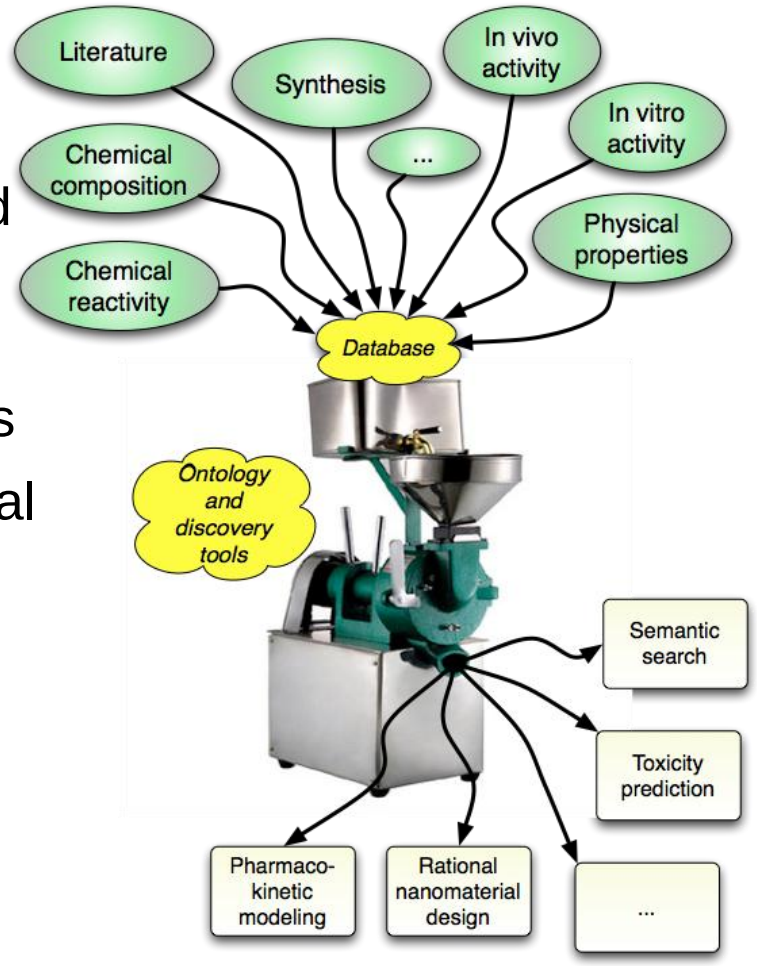
What does the community need?

- The nanomedicine community has an immediate need for nanomaterial informatics:
  - Understand nanomaterial toxicity and other biological properties
  - Search for existing data on nanoparticle synthesis and properties
  - Systematically represent nanomaterial structure and composition
  - Exchange nanomaterial chemical, physical, and biological data
  - Design nanoparticles, and other materials with custom properties for specific biological applications



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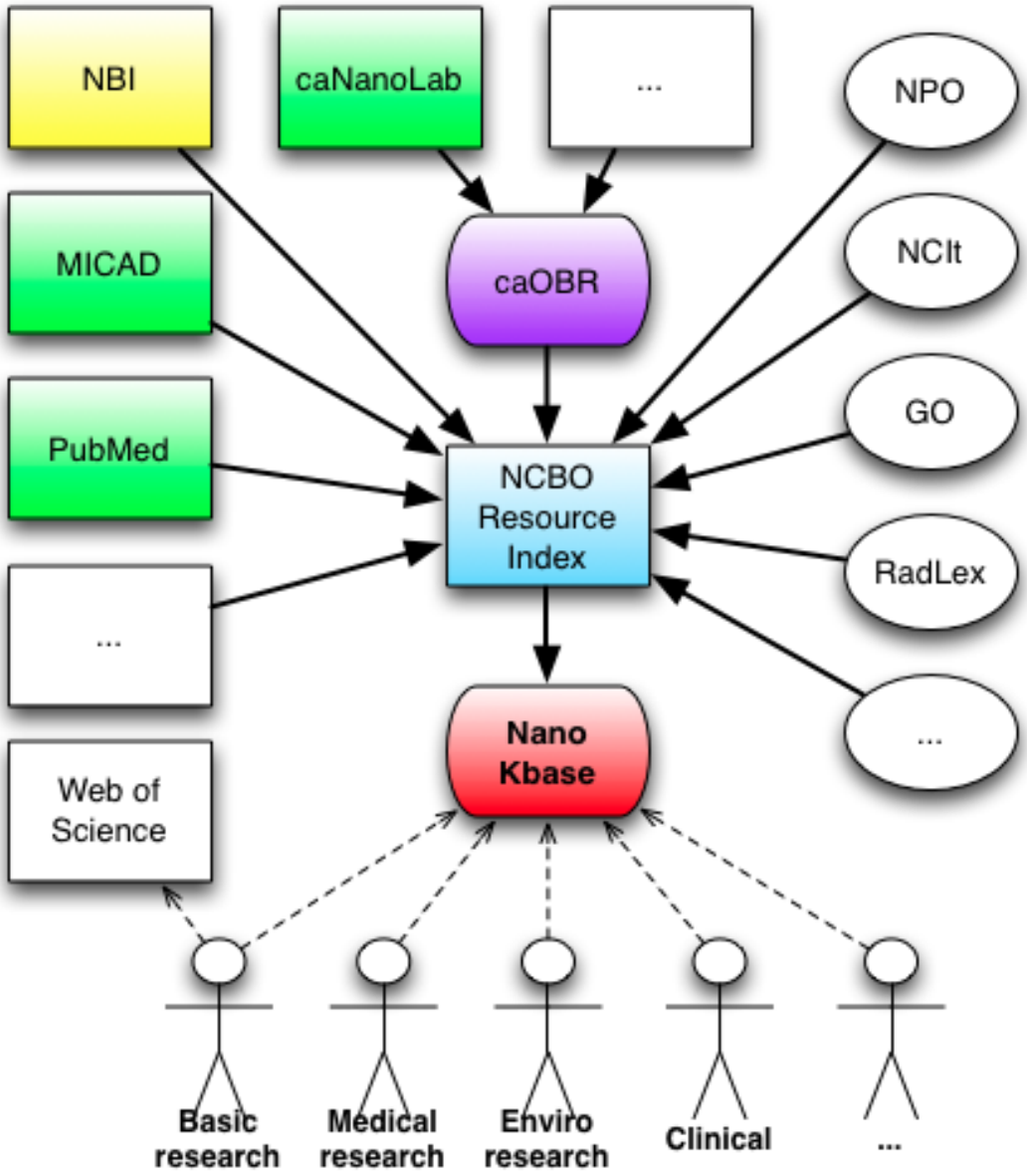
Our solution



- Information exchange and analysis through
  - Data exchange standards
  - Ontology
  - Information resources
- Methodology development and applications in nanomaterial prediction:
  - Biological activities
  - Chemical and physical characteristics

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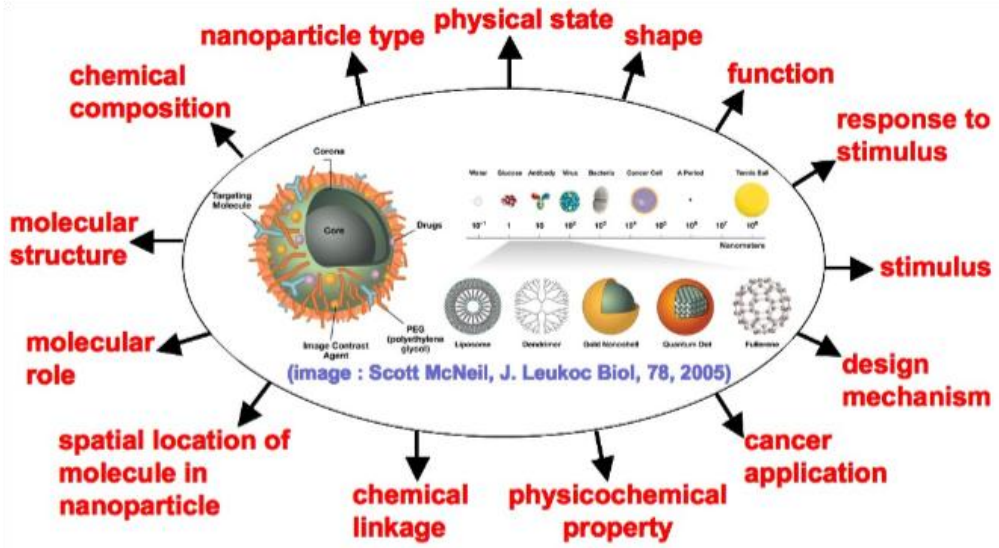
NanoParticle Ontology (NPO)

- Capture knowledge underlying nanomaterial
  - Preparation
  - Chemical composition
  - Physiochemical characterization
  - Biological function/behavior
- Basic Formal Ontology structure
- Initial focus on cancer diagnosis and therapy
- Current growth to include a broader range of nanotechnology concepts
- Supported by the caBIG® Nano WG
- Available through Bioportal



http://purl.bioontology.org/ontology/NPO

http://www.nano-ontology.org/

Thomas DG, Pappu RV, Baker NA. NanoParticle Ontology for Cancer Nanotechnology Research. *J Biomed Inform*, in press. doi:10.1016/j.jbi.2010.03.001

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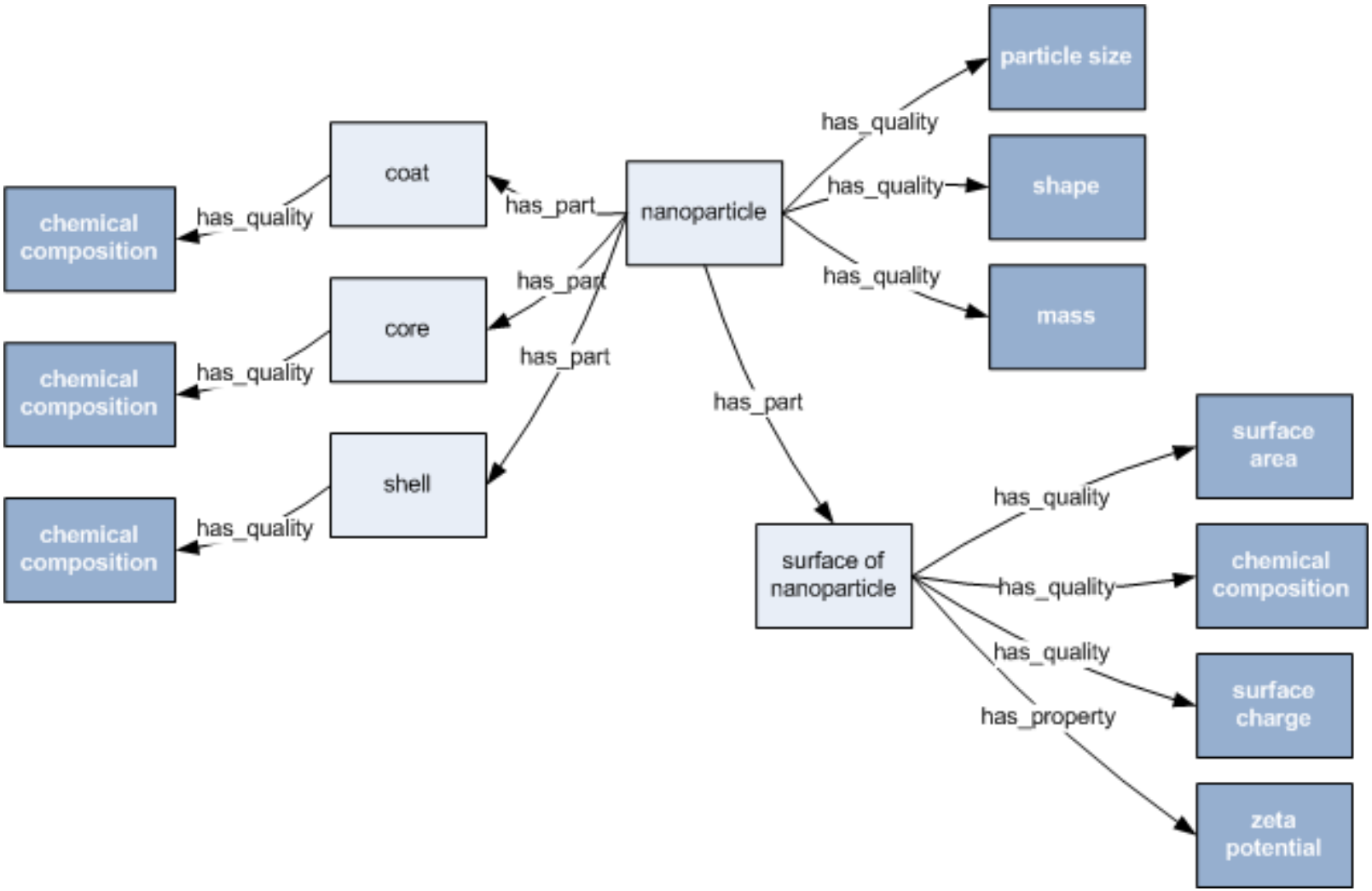
Example view into the NPO



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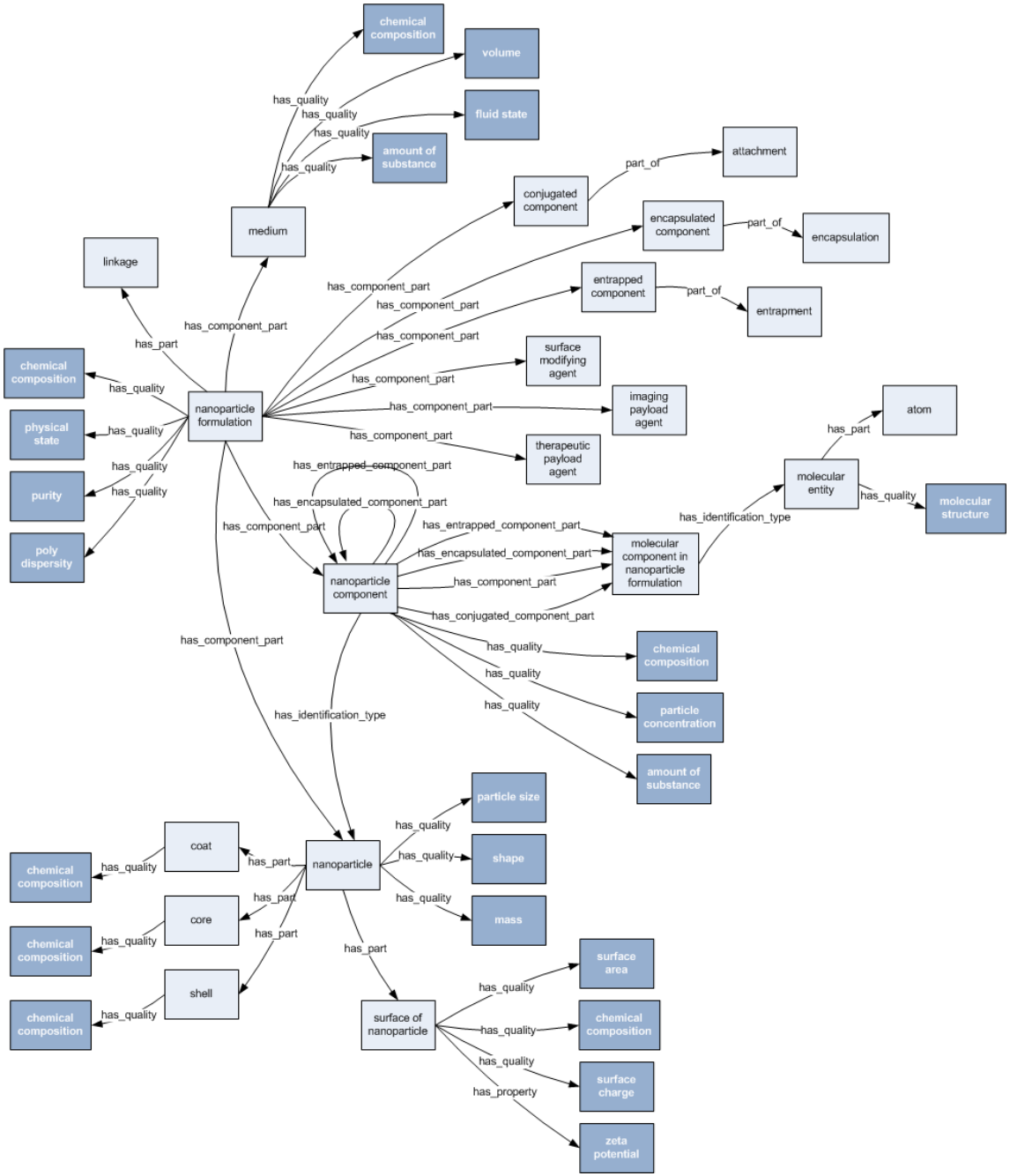
A more detailed view of nanoparticle composition using the NPO



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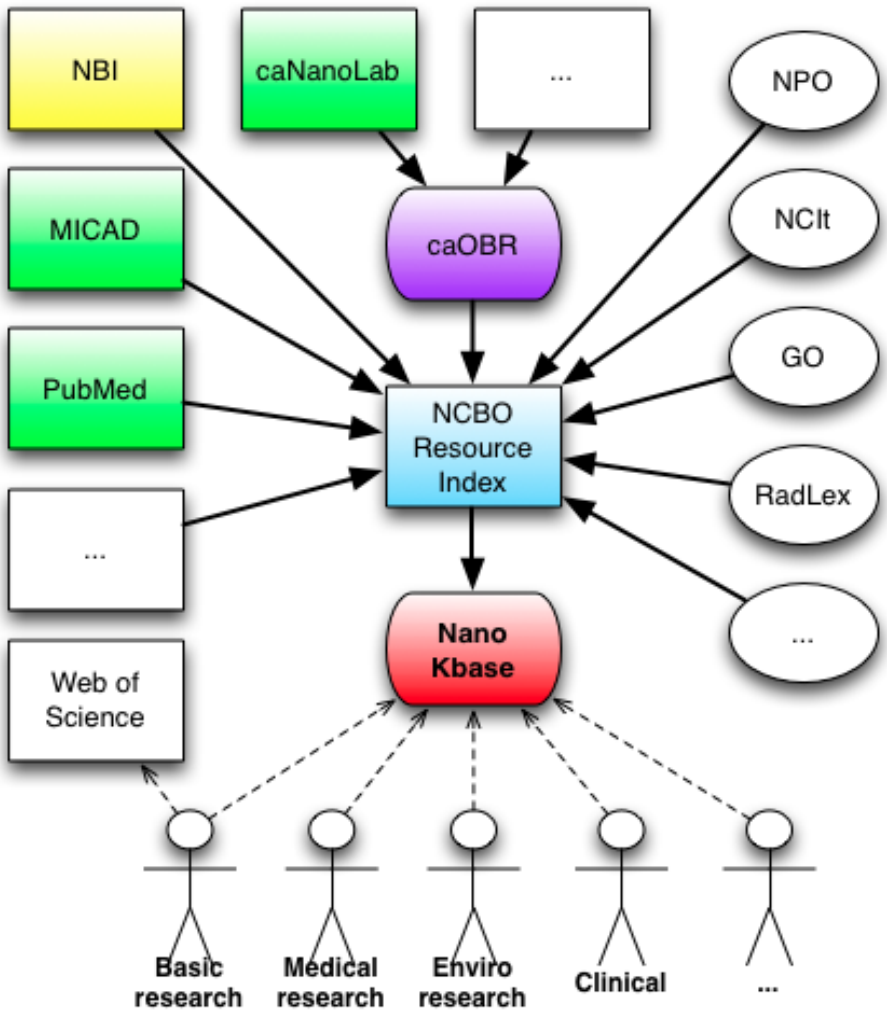
PubNano nanomedicine resource



- Nano-friendly interface to relevant:
  - Ontologies (browse and search)
  - Resources (semantic search)
  - Materials (structural search)
  - Literature (links back to relevant terminologies)
  - News
- Driven by:
  - NCBO Resource Index
  - Knowledge Encapsulation Framework (KEF)

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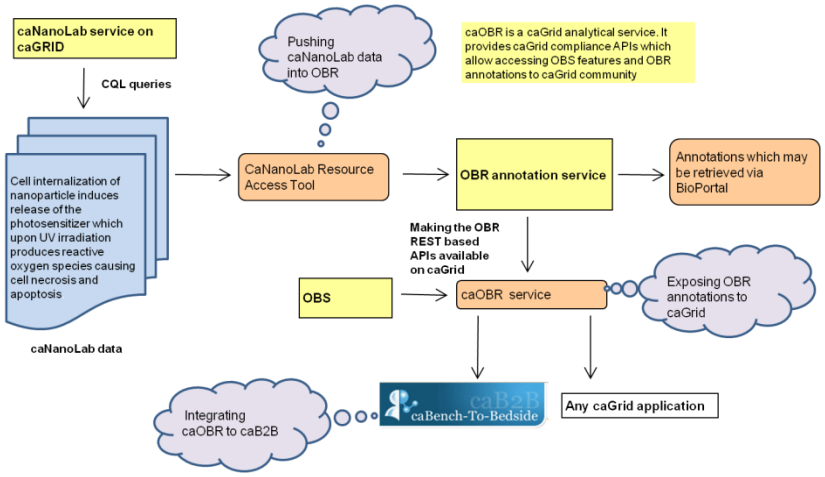
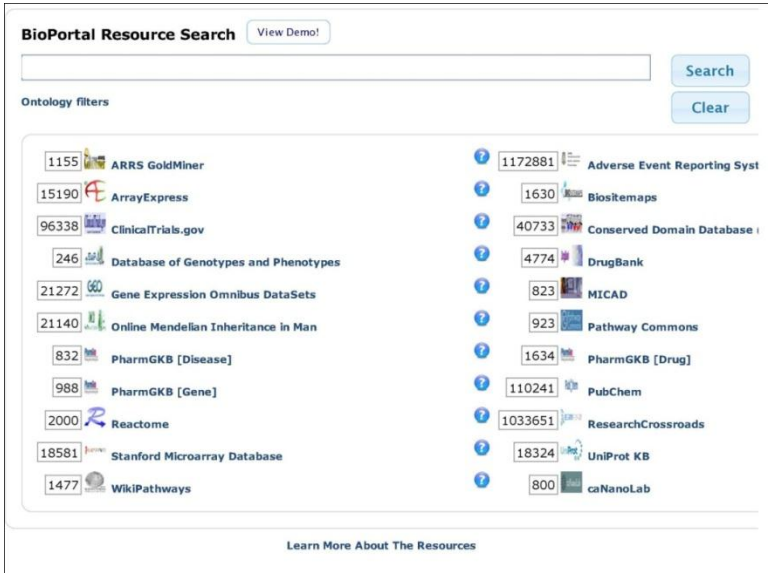
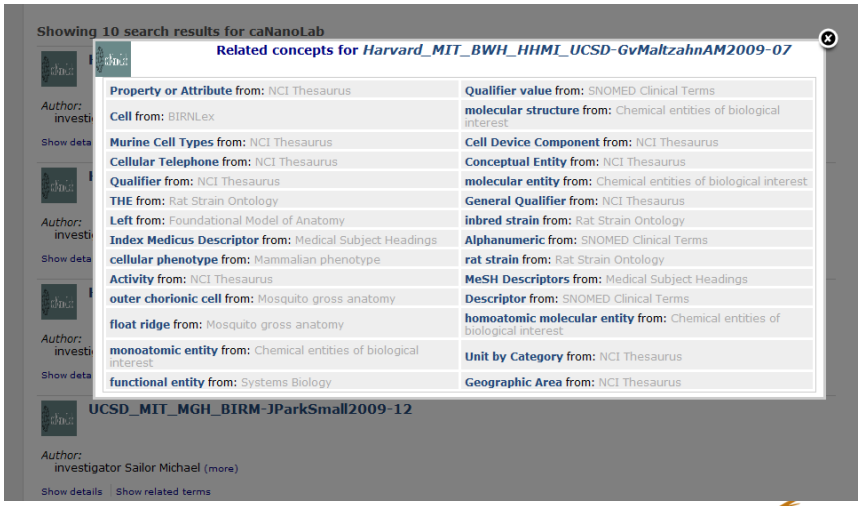
caOBR adds caBIG resources to the NCBO Resource Index

- caOBR: connecting caBIG with Bioportal
- Use the NPO and other ontologies for *semantic* search
- caOBR adds caBIG resources to NCBO Index
- caOBR also exposes NCBO Index to caBIG







NCBO BioPortal: http://bioportal.bioontology.org/

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KEF features: Semantic MediaWiki for annotation, search, and evidence marshalling

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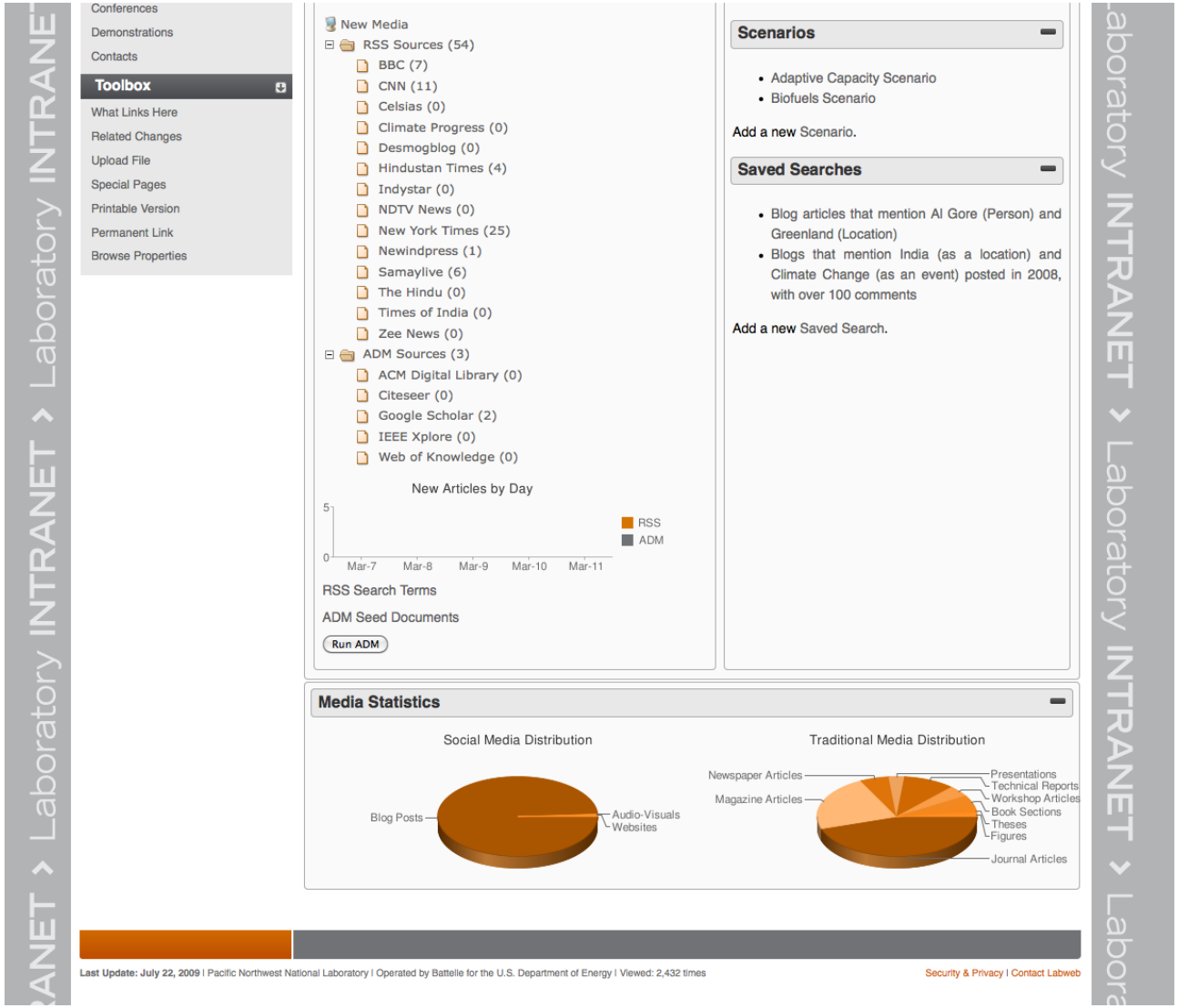

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PubNano: coming soon!

- Integration of:
  - PubMed
  - caNanoLab
  - MICAD
  - GEO
  - …
- Coming soon to http://pubnano.bioontology.org !

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NANO-TAB FOR NANOMATERIAL DATA SHARING

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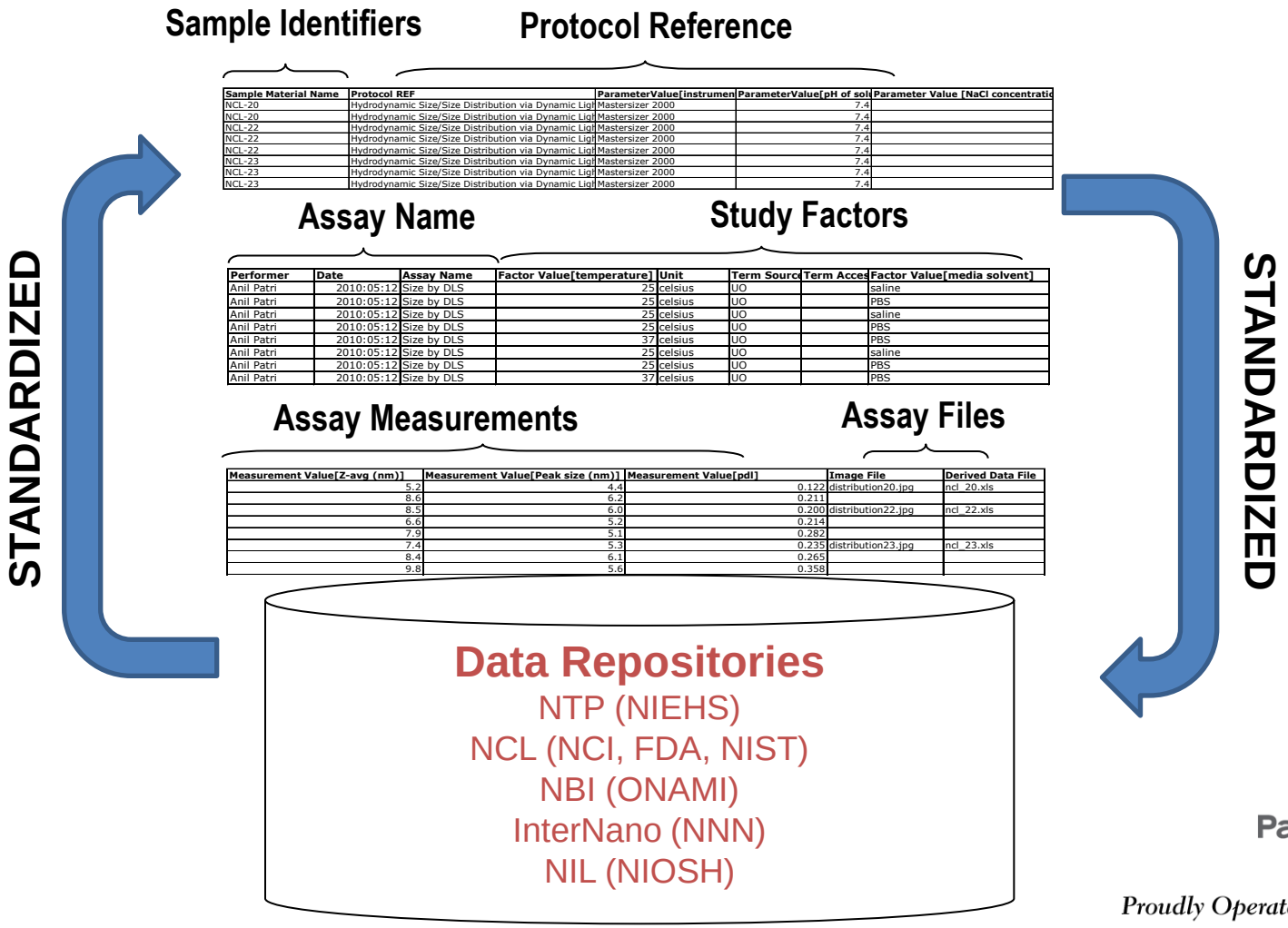
Target audiences and applications

- Audiences
  - Biomedical researchers
  - (Nano)-Materials scientists
  - Toxicologists
  - Regulatory scientists
  - Industrial hygienists
  - …
- Applications
  - Synthesis
  - Therapeutics, diagnostics, imaging
  - Bionics and prosthetics
  - Risk and exposure assessment
  - Toxicity prediction and reduction
  - Laboratory and occupational safety

Goal of nano-TAB

Develop a specification to facilitate the import/export of data on nanomaterials and their characterizations to/from nanotechnology resources



Sample Material Name	Protocol REF	ParameterValue[instrumen	ParameterValue[pH of sol	Parameter Value [NaCl concentratio
NCL-20	Hydrodynamic Size/Size Distribution via Dynamic Ligh	Mastersizer 2000	7.4	
NCL-20	Hydrodynamic Size/Size Distribution via Dynamic Ligh	Mastersizer 2000	7.4	
NCL-22	Hydrodynamic Size/Size Distribution via Dynamic Ligh	Mastersizer 2000	7.4	
NCL-22	Hydrodynamic Size/Size Distribution via Dynamic Ligh	Mastersizer 2000	7.4	
NCL-22	Hydrodynamic Size/Size Distribution via Dynamic Ligh	Mastersizer 2000	7.4	
NCL-23	Hydrodynamic Size/Size Distribution via Dynamic Ligh	Mastersizer 2000	7.4	
NCL-23	Hydrodynamic Size/Size Distribution via Dynamic Ligh	Mastersizer 2000	7.4	
NCL-23	Hydrodynamic Size/Size Distribution via Dynamic Ligh	Mastersizer 2000	7.4	

Performer	Date	Assay Name	Factor Value[temperature]	Unit	Term Source	Term Acces	Factor Value[media solvent]
Anil Patri	2010:05:12	Size by DLS	25	celsius	UO		saline
Anil Patri	2010:05:12	Size by DLS	25	celsius	UO		PBS
Anil Patri	2010:05:12	Size by DLS	25	celsius	UO		saline
Anil Patri	2010:05:12	Size by DLS	25	celsius	UO		PBS
Anil Patri	2010:05:12	Size by DLS	37	celsius	UO		PBS
Anil Patri	2010:05:12	Size by DLS	25	celsius	UO		saline
Anil Patri	2010:05:12	Size by DLS	25	celsius	UO		PBS
Anil Patri	2010:05:12	Size by DLS	37	celsius	UO		PBS

Measurement Value[Z-avg (nm)]	Measurement Value[Peak size (nm)]	Measurement Value[pdl]	Image File	Derived Data File
5.2	4.4	0.122	distribution20.jpg	ncl_20.xls
8.6	6.2	0.211		
8.5	6.0	0.200	distribution22.jpg	ncl_22.xls
6.6	5.2	0.214		
7.9	5.1	0.282		
7.4	5.3	0.235	distribution23.jpg	ncl_23.xls
8.4	6.1	0.265		
9.8	5.6	0.358		

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What is nano-TAB?

- A standard tab-delimited format for describing data related to
  - Investigations
  - Nanomaterials
  - Specimens
  - Assays
- 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
  - Example: MAGE-TAB
- Nano-TAB supports ontology-based curation
  - Nanomaterials and concepts from the NanoParticle Ontology (NPO) as well as other ontologies

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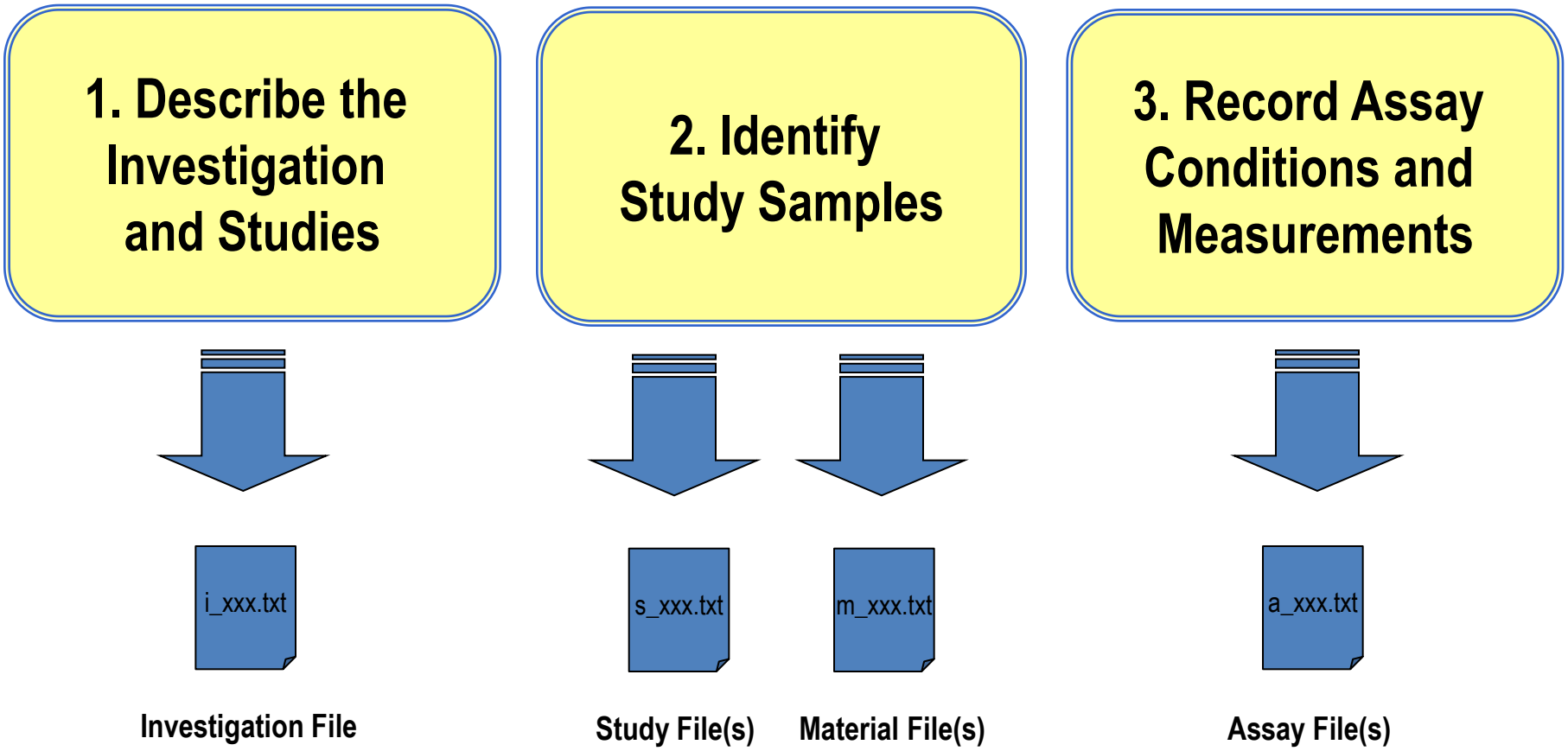
Uses and benefits

- Address the data sharing challenges in nanomedicine
- Provide a standard means for identifying nanomaterials and characterizations
- Enable the submission and exchange of nanomaterial data to/from nanotechnology data resources (e.g., NBI, caNanoLab, etc.)
- Empower organizations to adopt standards for representing data in nanotechnology publications
- Provide researchers with guidelines for representing nanomaterials and characterizations to achieve cross-material comparison

nano-TAB structure



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nano-TAB Investigation File

- Describes
  - Primary investigation
  - Associated studies, assays, and protocols
- Descriptive information about the study includes
  - Design descriptors and factors
  - Publications
  - Assays and protocols
  - Contacts
- Vertical-based spreadsheet format with columns representing multiple values

Investigation File

ONTOLOGY SOURCE REFERENCE		
Term Source Name	MO	NPO
Term Source File		
Term Source Version	v1.0	v1.0
Term Source Description	MGED Ontology	Nanoparticle Ontology
INVESTIGATION		
Investigation Identifier	NCL200612A	
Investigation Title	Dendrimer-Based MRI Contrast Agents	
Investigation Description	The objective of the Dendritic Nanotechnologies, Inc. - NCL collaboration is to characterize a PAMAM dendrimer with an associated gadolinium chelate MRI contrast agent. The nanomaterials submitted for testing at the NCL were (NCL20) G4 tris (hydroxyl) terminated PAMAM dendrimer, (NCL21) G4 pyrrolidinone terminated PAMAM dendrimer, (NCL22) G4.5 CDONs terminated PAMAM dendrimer, (NCL23) G4.5 CDONs terminated PAMAM dendrimer-Magnevist/E complex, (NCL25) G4 tris (hydroxyl) terminated PAMAM dendrimer-Magnevist/E complex, and (NCL26) G4 pyrrolidinone terminated PAMAM dendrimer-Magnevist/E complex. Commercially available Magnevist/E (NCL24) was used as a control. NCL studies addressed in this report can be divided into three main categories: physicochemical characterization; immunotoxicology; in vitro toxicology.	
Investigation Disease		
Investigation Disease Term Accession Number		
Investigation Disease Term Source REF		
Investigation Outcome		
Investigation Submission Date	12/1/2006	
Investigation Public Release Date	12/1/2006	
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	peer reviewed	
Investigation Publication Status Term Accession Number		
Investigation Publication Status Term Source REF	NPO	
INVESTIGATION CONTACTS		
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Investigation Person Fax		
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Investigation Person Affiliation	Nanotechnology Characterization Laboratory	Nanotechnology Characte
Investigation Person Roles	investigator	investigator
Investigation Person Roles Term Accession Number		
Investigation Person Roles Term Source REF	MO	MO

Ontology References

Investigation Description

Publications

Contacts

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Investigation File (cont.)

STUDY	
Study Identifier	NCL200612A-SIZE
Study Title	Size by DLS
Study Submission Date	Dec-06
Study Public Release Date	Dec-06
Study Description	Dynamic light scattering (DLS) technique was used to measure the hydrodynamic size of this dendritic nanomaterial. The effects of sample concentration, buffer, and temperature on the hydrodynamic size (stability) also were measured. Purity was analyzed by HPLC and Capillary Electrophoresis. MALDI-TOF Mass spectrometry was used to obtain the molecular weight information and to determine the purity, existence of dimers, trimers, and trailing generations in the sample. Gadolinium quantitation, which is important to determine the relaxivity as a MRI contrast agent, was carried out by Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES). Fractionation methods such as Size Exclusion Chromatography (SEC) and Asymmetric-flow Field Flow Fractionation (AFFF) were used to determine the molecular weight information as well as purity. Finally, a 3T clinical MRI machine was used to obtain relaxivity measurements on this sample to compare with free MagnevistÆ. No significant relaxivity change was observed upon association of MagnevistÆ with the dendrimer.
Study Disease	
Study Disease Term Accession Number	
Study Disease Term Source REF	
Study Outcome	For NCL22, the size is slightly larger when dispersed in saline compared to PBS. In PBS, the size is independent of temperature. This is in contrast to NCL23, which is larger in PBS than in saline. NCL23 also shows temperature dependence, as its size decreases slightly with increased temperature in PBS. Finally, NCL20 is larger when dispersed in PBS compared to saline.
STUDY SAMPLES	
Study Sample File Name	m_NCL-21.txt; m_NCL-22.txt; m_NCL-23.txt
Study Sample File URI	
Study Sample File Type	material sample; material sample; material sample
Study Sample File Type Term Accession Number	
Study Sample File Type Term Source REF	
Study Sample File Version	
Study Sample File Description	
STUDY DESIGN DESCRIPTORS	
Study Design Type	comparison
Study Design Type Term Accession Number	
Study Design Type Term Source REF	
STUDY PUBLICATIONS	
Study PubMed ID	
Study Publication DOI	
Study Publication Author list	
Study Publication Title	
Study Publication Status	
Study Publication Status Term Accession Number	
Study Publication Status Term Source REF	

Study Description

Sample Files

Design

Publication

Pacific Northwest
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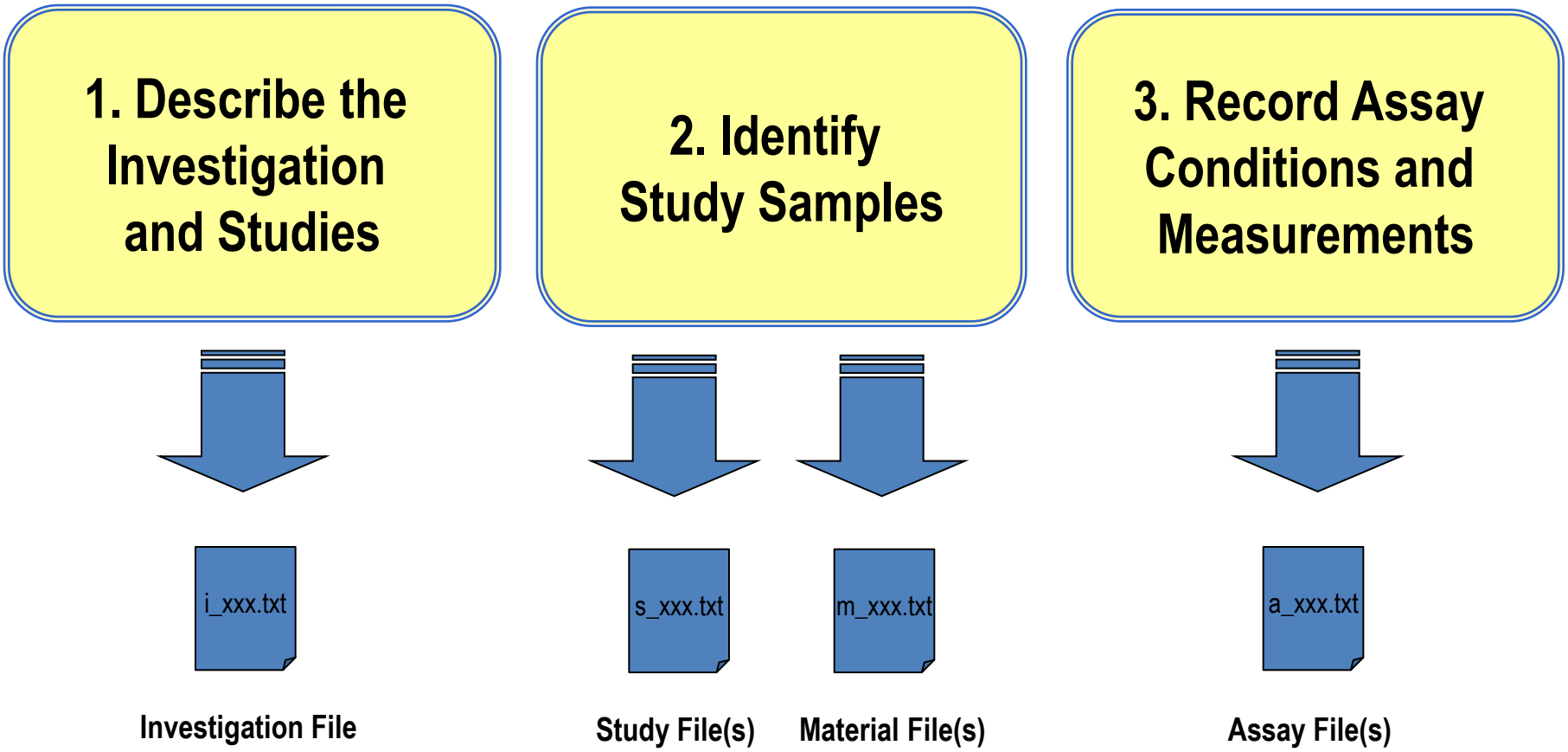
nano-TAB structure



nano-TAB Study File

- Study files provide mappings between the samples, materials, and processing events associated with a study.
- Samples can be
  - Biological materials
  - Nanomaterials
  - Small molecules
- For physical-chemical characterizations of nanomaterials, the sample is the nanomaterial.
- For in vitro and in vivo characterizations, the sample is the biological specimen (cell line, animal, etc.)

nano-TAB Material File

- Primary file for describing
  - Nanomaterial composition and formulation
  - Physical properties
  - Structure
- Allows for
  - Comparison of nanomaterials across nanotechnology resources
  - Association with optional files; e.g., a Structure file for representing the 3D structure of the nanomaterial
- Vertical-based spreadsheet with the following sections:
  - MATERIAL SAMPLE
  - MATERIAL COMPONENT
  - MATERIAL LINKAGE

Material File

Material Sample Section

Material Identifiers

Material Characteristics

Material Files

MATERIAL SAMPLE			
Material Sample Source Name	NCL-23		
Material Sample Name	NCL-23-F1		
Material Sample Type	nanoparticle sample		
Material Sample Type Term Accession Number	NPO_1404		
Material Sample Type Term Source REF	NPO		
Material Sample Description	G4.5 COONa terminated PAMAM dendrimer-MagnevistÂ® complex		
Material Sample Synthesis			
Material Sample Design Rationale			
Material Sample Design RationaleTerm Accession Number			
Material Sample Design Rationale Term Source REF			
Material Sample Characteristic			
Material Sample Characteristic Term Accession Number			
Material Sample Characteristic Term Source REF			
Material Sample Characteristic Value			
Material Sample Characteristic Value Term Accession Number			
Material Sample Characteristic Value Term Source REF			
Material Sample Characteristic Statistic			
Material Sample Characteristic Statistic Term Accession Number			
Material Sample Characteristic Statistic Term Source REF			
Material Sample Characteristic Unit			
Material Sample Characteristic Unit Term Accession Number			
Material Sample Characteristic Unit Term Source REF			
Material Sample Intended Application	MRI Contrast Agent		
Material Sample Intended Application Term Accession Number	NPO_581		
Material Sample Intended Application Term Source REF	NPO		
Material Sample File Name	ncl-23_composition.png; ncl-23_structure.pdb		
Material Sample File Location			
Sampe Material File Type	image; structure		
Material Sample File Type Term Accession Number			
Material Sample File Type Term Source REF			
Material Sample File Version	1.0; 1.0		
Material Sample File Description	NCL23 composition schematic; 3D structure of the dendrimer with annotated voids		

Material File

Material Component Section

Material Component Identifier

Material Component Characteristics

Material Component Files

MATERIAL COMPONENT			
Material Component Name	NCL-23-F1-N1	NCL-23-F1-N1-M1	NCL-23-F1-N1-M2
Material Component Type	dendrimer	core	small molecule
Material Component Type Term Accession Number	NPO_735	NPO_279	
Material Component Type Term Source REF	NPO	NPO	
Material Component Description			
Material Component Chemical Name		diaminobutane	magnevist
Material Component Chemical Term Accession Number			CHEBI.31797
Material Component Chemical Term Source REF			CHEBI
Material Component Characteristic	branch; generation		amount; molecular formula
Material Component Characteristic Term Accession Number	NPO_776; NPO_224		NPO_1217;
Material Component Characteristic Term Source REF	NPO; NPO		NPO;
Material Component Characteristic Value	1-4; 4.5		0; [Gd+3] .CNC[C@H] (O) [C@@H] (O) [C@H] (O) [C@H] (O) CO.CNC[C@H] (O) [C@@H] (O) [C@H] (O) [C@H] (O) CO.OC(=O) CN(CCN(CCN(CC(O) =O) CC([O-]) =O) CC([O-]) =O) CC([O-]) =O
Material Component Characteristic Value Term Accession Number			
Material Component Characteristic Value Term Source REF			
Material Component Characteristic Statistic			
Material Component Characteristic Statistic Term Accession Number			
Material Component Characteristic Statistic Term Source REF			
Material Component Characteristic Unit			mL; SMILES
Material Component Characteristic Unit Term Accession Number			UO_0000101;
Material Component Characteristic Unit Term Source REF			UO;
Material Component Intended Application			MRI Contrast Agent
Material Component Intended Application Term Accession Number			NPO_581
Material Component Intended Application Term Source REF			NPO
Material Component File Name			magnevist_structure.png
Material Component File Type			image
Material Component File Type Term Accession Number			
Material Component File Type Term Source REF			
Material Component File Version			

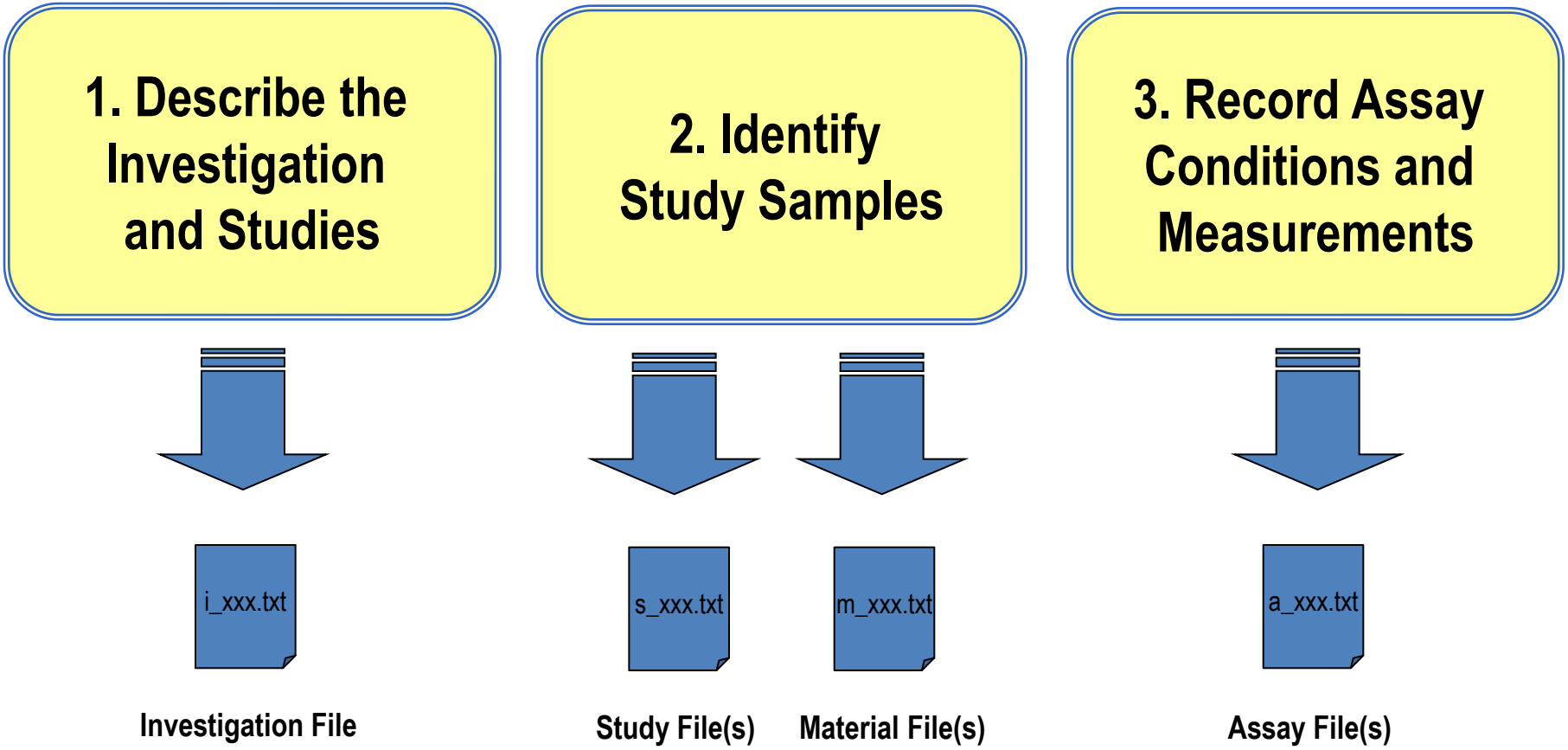
Material File
Material Linkage Section

Material Linkage Identifier

Material Linkage Characteristics

MATERIAL LINKAGE			
Material Linkage Name	NCL-23-F1-L1		
Material Linkage Type	association		
Material Linkage Type Term Accession Number			
Material Linkage Type Term Source REF			
Material Linkage Component A	NCL-23-F1-N1-M1		
Material Linkage Component B	NCL-23-F1-N1-M2		
Material Linkage Component Location	exterior dendrimer surface		
Material LinkageComponent Location Term Accession Number			
Material Linkage Component Location Term Source REF			
Material Linkage Characteristic	bond type		
Material Linkage Characteristic Term Accession Number			
Material Linkage Characteristic Term Source REF			
Material Linkage Characteristic Value			
Material Linkage Characteristic Value Term Accession Number			
Material Linkage Characteristic ValueTerm Source REF			
Material Linkage Characteristic Statistic			
Material Linkage Characteristic Statistic Term Accession Number			
Material Linkage Characteristic Statistic Term Source REF			
Material Linkage Characteristic Unit			
Material Linkage Characteristic Unit Term Accession Number			
Material Linkage Characteristic Unit Term Source REF			

nano-TAB structure



nano-TAB Assay File

- Describes the protocol parameters and factors, including:
  - Temperature
  - Media/solvent
  - Concentration
- Provides references or links to assay results, including:
  - Measurements
  - Instrumentation
  - Derived data files
- Templates available for the “top Nano WG assays”
  - Size by DLS (Physico-Chemical)
  - Zeta Potential (Physico-Chemical)
  - Hemolysis (In Vitro)
  - Hepatocarcinoma Cytoxicity (MTT and LDH) (In Vitro)
  - Caspase 3 Apoptosis (In Vitro)
  - Toxicity (ADME, Single/Repeat Dose) (In Vivo)
  - ***Your assay here!***

nano-TAB Assay File

- Horizontal-based spreadsheet format with the following sections:
  - SAMPLE NAMES
  - PARAMETERS
  - FACTORS
  - ASSAY MEASUREMENTS
  - ASSAY FILES

Assay File
Size by DLS

Sample Identifiers

Protocol Reference

Material Sample Name	Protocol REF	ParameterValue[pH of solutio	Parameter Value [NaCl concentration	Performer	Date
NCL-20-F1	Hydrodynamic Size/Size Distribution via Dynamic Ligh	7.4		Anil Patri	2010:05:12
NCL-20-F1	Hydrodynamic Size/Size Distribution via Dynamic Ligh	7.4		Anil Patri	2010:05:12
NCL-22-F1	Hydrodynamic Size/Size Distribution via Dynamic Ligh	7.4		Anil Patri	2010:05:12
NCL-22-F1	Hydrodynamic Size/Size Distribution via Dynamic Ligh	7.4		Anil Patri	2010:05:12
NCL-22-F1	Hydrodynamic Size/Size Distribution via Dynamic Ligh	7.4		Anil Patri	2010:05:12
NCL-23-F1	Hydrodynamic Size/Size Distribution via Dynamic Ligh	7.4		Anil Patri	2010:05:12
NCL-23-F1	Hydrodynamic Size/Size Distribution via Dynamic Ligh	7.4		Anil Patri	2010:05:12
NCL-23-F1	Hydrodynamic Size/Size Distribution via Dynamic Ligh	7.4		Anil Patri	2010:05:12

Assay Name

Study Factors

Assay Name	Factor Value[temperature]	Unit	Term Source	Term Acces	Factor Value[media solvent]	Measurement Value[size]	Statistic	Unit	Term Source
Size by DLS	25	celsius	UO		saline	5.2	z-average	nm	UO
Size by DLS	25	celsius	UO		PBS	8.6	z-average	nm	UO
Size by DLS	25	celsius	UO		saline	8.5	z-average	nm	UO
Size by DLS	25	celsius	UO		PBS	6.6	z-average	nm	UO
Size by DLS	37	celsius	UO		PBS	7.9	z-average	nm	UO
Size by DLS	25	celsius	UO		saline	7.4	z-average	nm	UO
Size by DLS	25	celsius	UO		PBS	8.4	z-average	nm	UO
Size by DLS	37	celsius	UO		PBS	9.8	z-average	nm	UO

Assay Measurements

Assay Files

Term Acces	Measurement Value[Peak size]	Unit	Term Source	Term Acces	Measurement Value[pdl]	Image File	Derived Data File
	4.4	nm	UO		0.122	distribution20.jpg	ncl_20.xls
	6.2	nm	UO		0.211		
	6.0	nm	UO		0.200	distribution22.jpg	ncl_22.xls
	5.2	nm	UO		0.214		
	5.1	nm	UO		0.282		
	5.3	nm	UO		0.235	distribution23.jpg	ncl_23.xls
	6.1	nm	UO		0.265		
	5.6	nm	UO		0.358		

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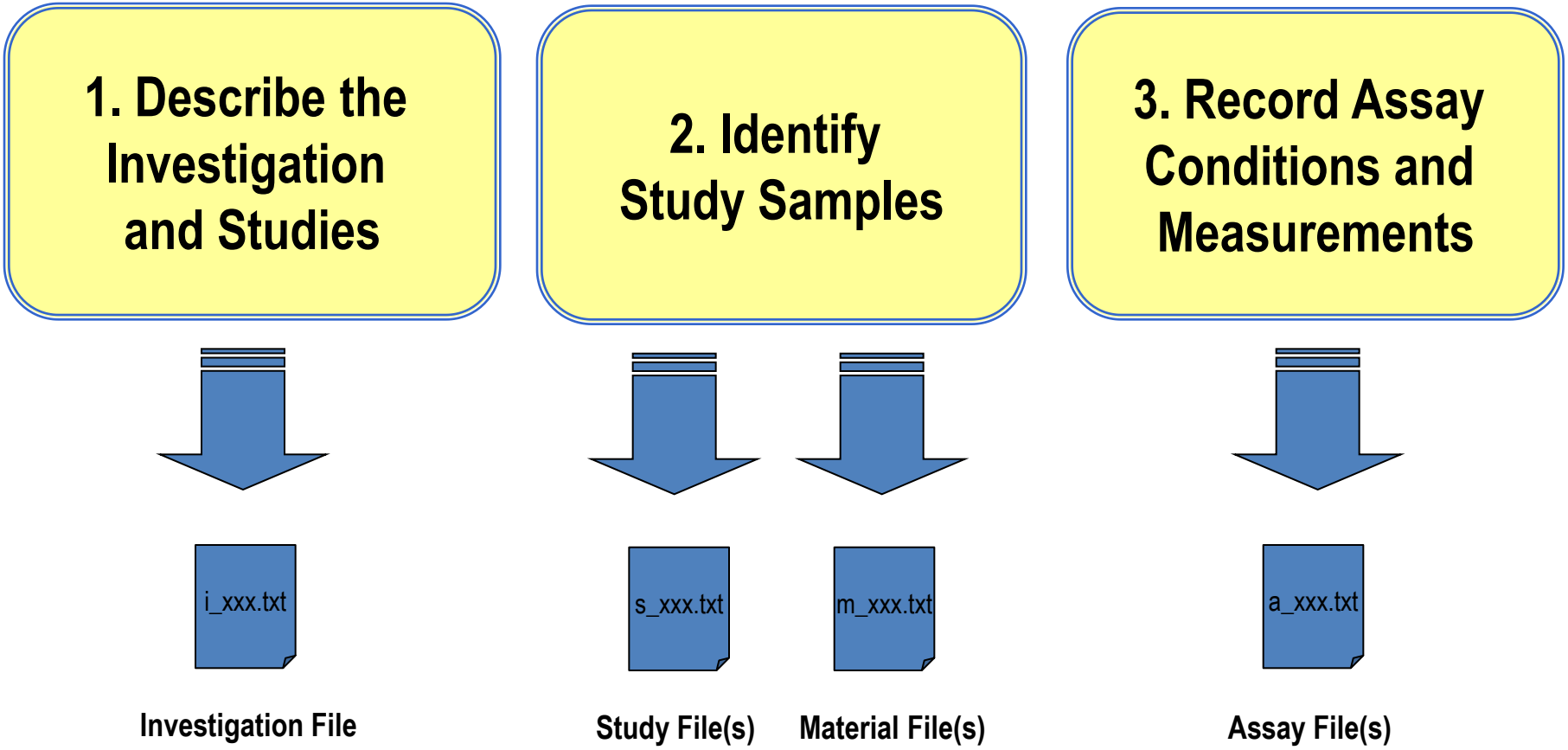

Getting Started

1. Contact us for help! nano-tab-l@list.nih.gov
2. Use nano-TAB template to create nano-TAB files: http://goo.gl/T7Mwi
3. Leverage template glossary for definitions: http://goo.gl/YkRZM
4. View example files: http://goo.gl/yKFew
5. Navigate the BioPortal ontology for terms: http://goo.gl/SVmNZ
6. Complete nano-TAB files and send to the nano-TAB Listserv: nano-tab-l@list.nih.gov

caBIG® Nano WG nano-TAB Site:
http://goo.gl/yKFew

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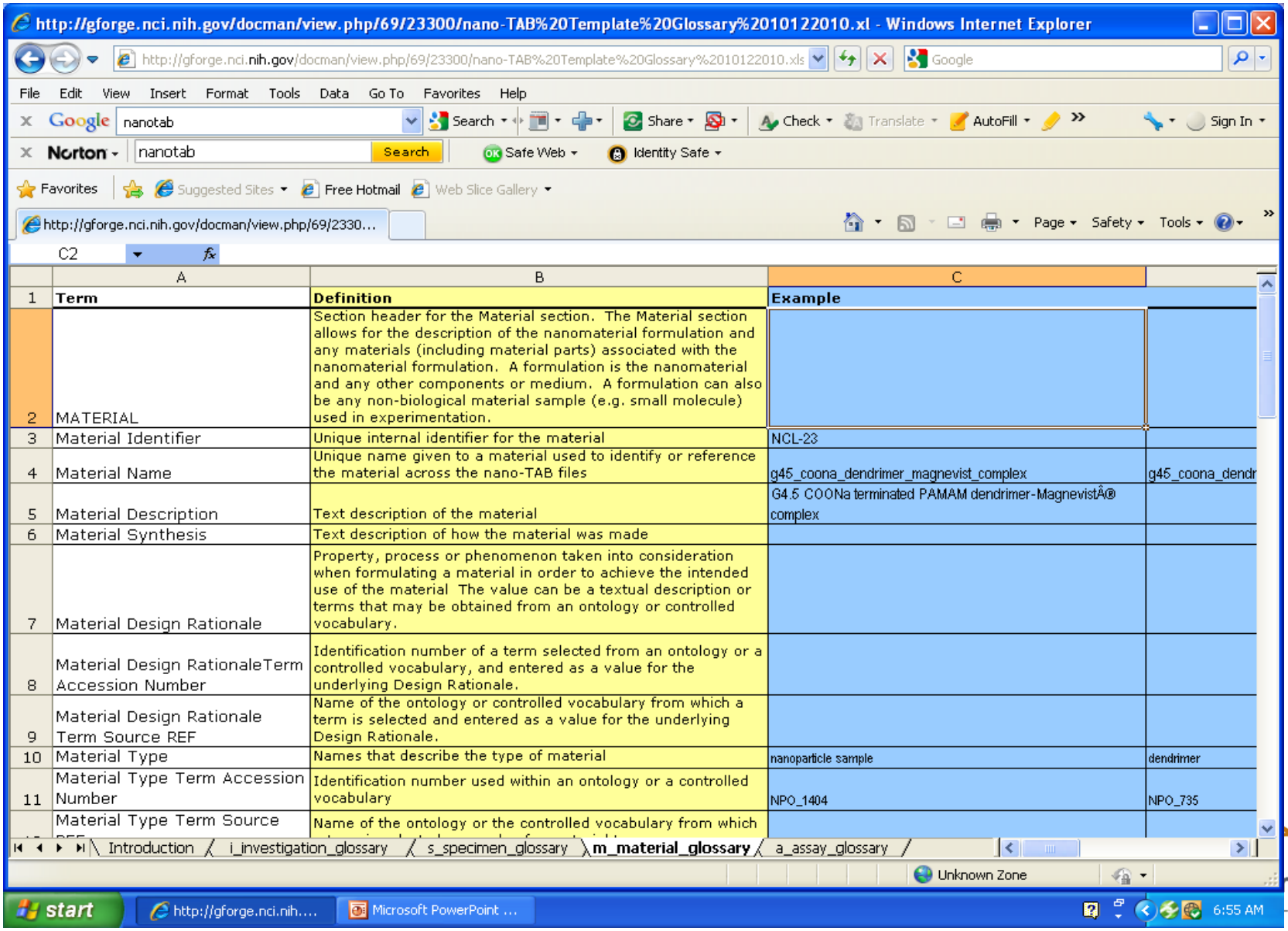
nanoTAB Template Glossary



	A	B	C	
1	**Term**	**Definition**	**Example**	
2	MATERIAL	Section header for the Material section. The Material section allows for the description of the nanomaterial formulation and any materials (including material parts) associated with the nanomaterial formulation. A formulation is the nanomaterial and any other components or medium. A formulation can also be any non-biological material sample (e.g. small molecule) used in experimentation.		
3	Material Identifier	Unique internal identifier for the material	NCL-23	
4	Material Name	Unique name given to a material used to identify or reference the material across the nano-TAB files	g45_coona_dendrimer_magnevist_complex	g45_coona_dendr
5	Material Description	Text description of the material	G4.5 COONa terminated PAMAM dendrimer-MagnevistÂ® complex	
6	Material Synthesis	Text description of how the material was made		
7	Material Design Rationale	Property, process or phenomenon taken into consideration when formulating a material in order to achieve the intended use of the material The value can be a textual description or terms that may be obtained from an ontology or controlled vocabulary.		
8	Material Design RationaleTerm Accession Number	Identification number of a term selected from an ontology or a controlled vocabulary, and entered as a value for the underlying Design Rationale.		
9	Material Design Rationale Term Source REF	Name of the ontology or controlled vocabulary from which a term is selected and entered as a value for the underlying Design Rationale.		
10	Material Type	Names that describe the type of material	nanoparticle sample	dendrimer
11	Material Type Term Accession Number	Identification number used within an ontology or a controlled vocabulary	NPO_1404	NPO_735
	Material Type Term Source	Name of the ontology or the controlled vocabulary from which		

nano-TAB future

- ASTM ballot
- User guide
  - Basic descriptions of elements, glossary
  - Organized collection of examples
  - Tutorials
- Easier NPO annotation and integration
  - List of most relevant terms
  - List of missing terms
- Real world applications
  - “Client” engagement
  - Friendly user support

http://cananolab.nci.nih.gov/caNanoLab/welcome.do

http://nbi.oregonstate.edu/knowledgebase

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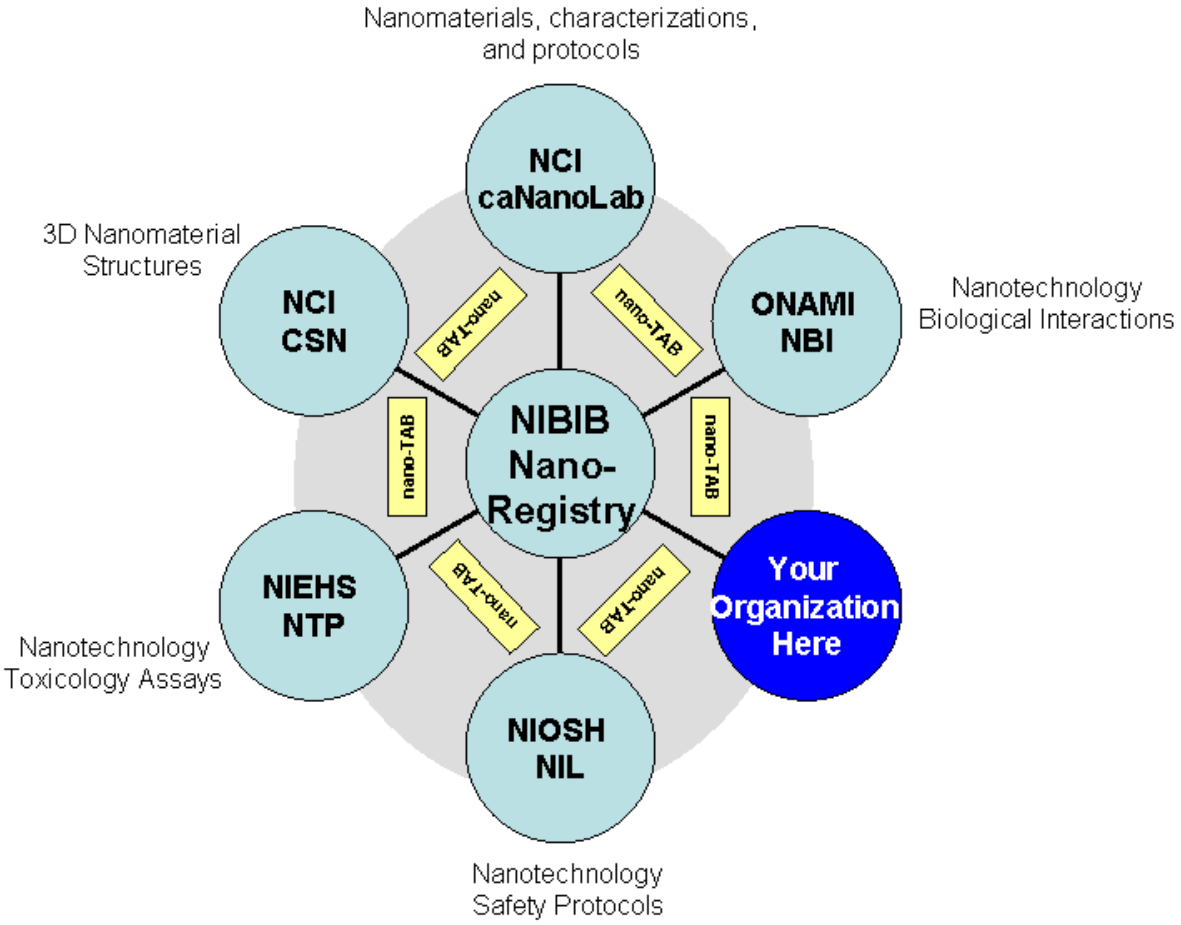
nano-TAB is a community-driven effort



Additional nano-TAB reading and project team

- nano-TAB Project Site: http://goo.gl/yKFew
- ASTM nano-TAB Work Item WK28974: http://goo.gl/OjSOX
- ISA-TAB: http://isatab.sourceforge.net
- caBIG ICR Nano WG Data Standards Document: http://goo.gl/sDEvp
- NanoParticle Ontology (NPO): http://www.nano-ontology.org

Nano-TAB project team

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Juli Klemm, NCI CBIIT
David Paik, Stanford University
Sue Pan, SAIC
Grace Stafford, The Jackson Laboratory
Todd Stokes, Georgia Tech
Dennis Thomas, PNNL

Summary

- Introduction to the caBIG® Nanotechnology Working Group
- Overview of nanotechnology informatics challenges
- Research projects
  - Ontology development
  - PubNano resource
  - Data exchange standards
  - Structure-property-activity modeling

Collaborators

caBIG® ICR Workspace, NCBO staff, ASTM, Raul Cachau, Gilbert Fragoso, Elaine Freund, Marty Fritts, Sam Gambhir, Sharon Gaheen, Liz Hahn-Dantona,Stacey Harper, Mark Hoover, Fred Klaessig, Juli Klemm, Michal Lijowski, David Paik, Sue Pan, Rohit Pappu, Persistent Systems Ltd, Daniel Rubin, Stan Shaw, Dennis Thomas, Eddie Xu, Kilian Weinberger, Trish Whetzel, …and many more!

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