NATIONAL CANCER INSTITUTE
Office of Cancer Nanotechnology Research

NCI Alliance for Nanotechnology in Cancer

caNanoLab Data Portal Overview

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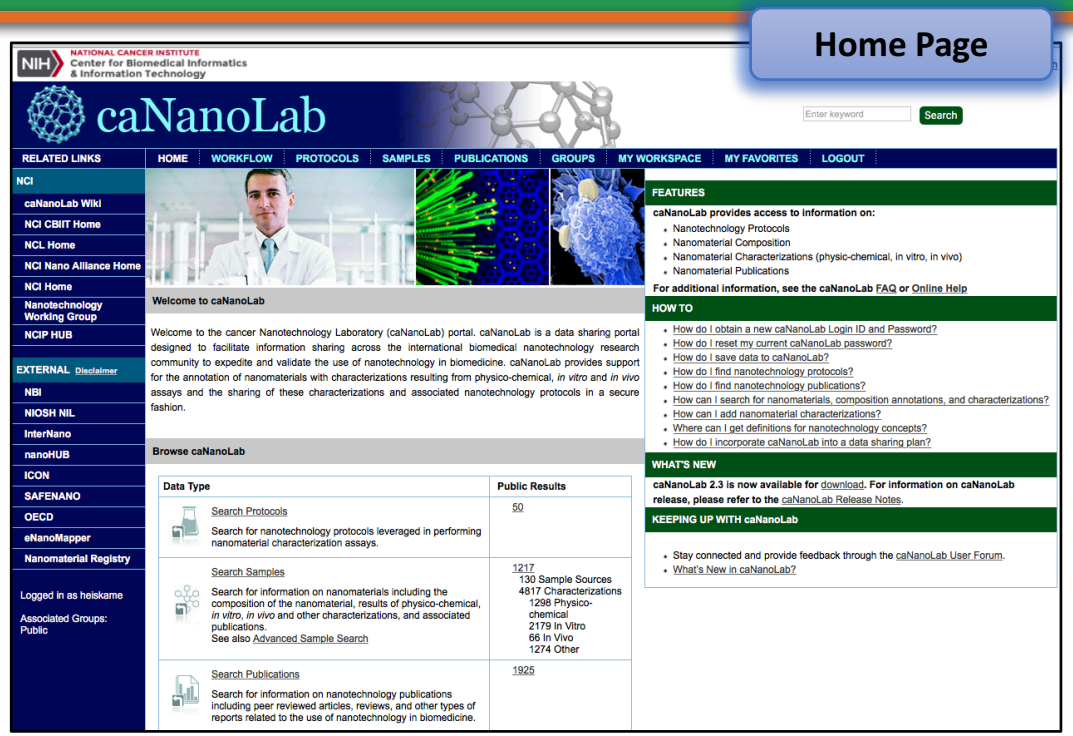
June 30, 2017
NIEHS NHIR Meeting

caNanoLab Data Portal: A Resource for Data Sharing



caNanoLab Goal

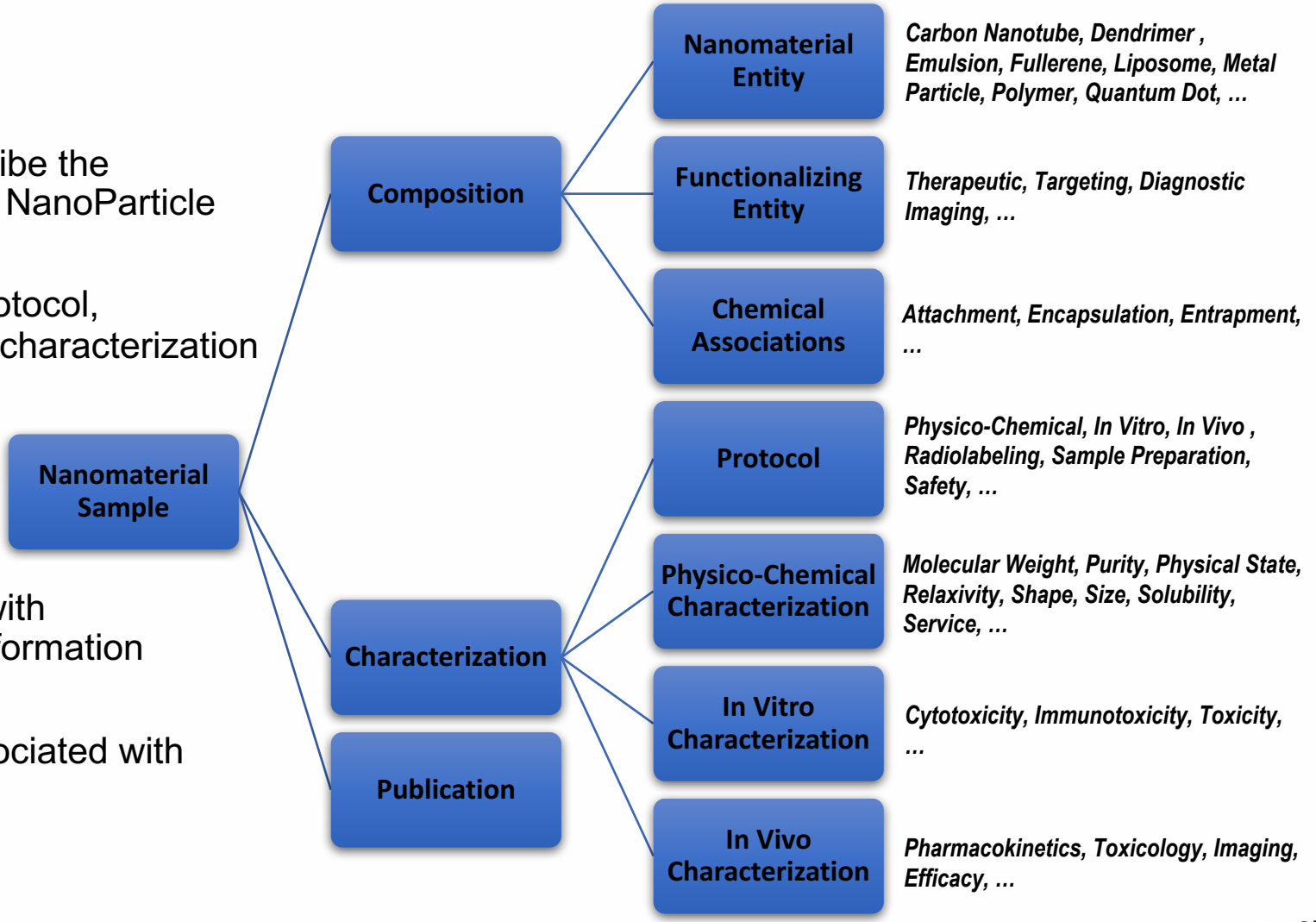
To provide a nanotechnology resource that facilitates data sharing in the community to expedite and validate the use of nanomaterials in biomedicine

https://cananolab.nci.nih.gov

- Provides support for the annotation of nanomaterials with composition information, and physico-chemical, *in vitro*, and *in vivo* characterizations
- Provides access to nanomaterial information, protocols, and publications from the NCI Nanotechnology Characterization Laboratory (NCL), NCI Alliance for Nanotechnology in Cancer, and the broader biomedical nanotechnology community

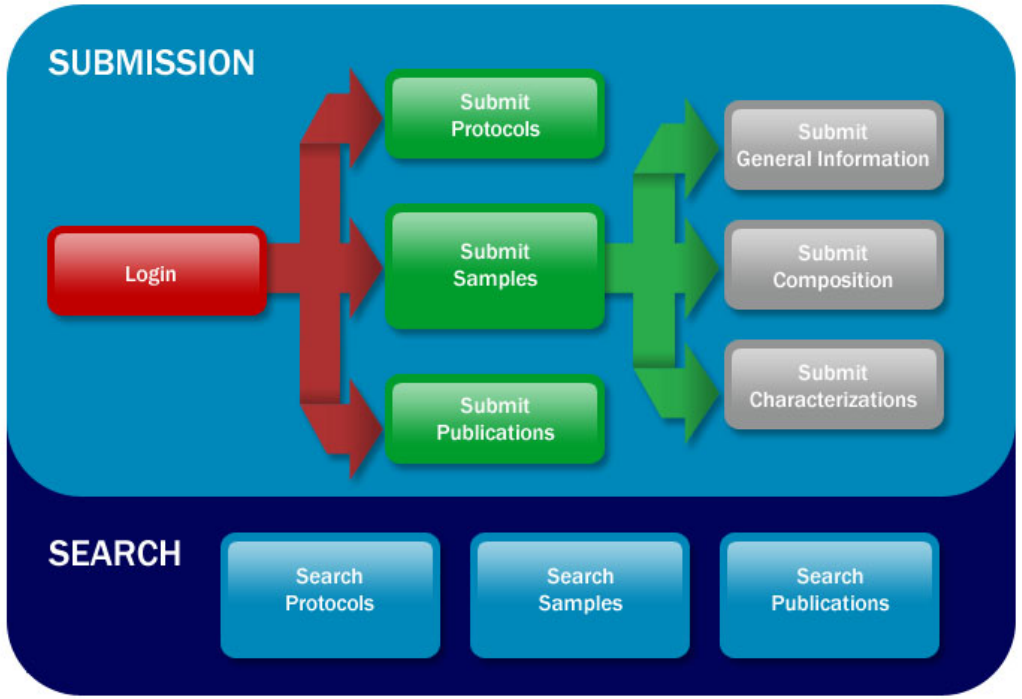
caNanoLab High-Level Concepts

- caNanoLab maintains metadata to describe the composition of each particle type; use of NanoParticle Ontology
- For characterizations, can specify the protocol, instruments, and techniques used in the characterization assay
- Submitted protocols can be associated with characterizations during nanomaterial information submission
- Similarly, submitted samples can be associated with publications



Gaheen et al., 2013, *Comput Sci Discov;*
Morris et al., 2015, *Beilstein J Nanotechnol*

caNanoLab Curation and Content

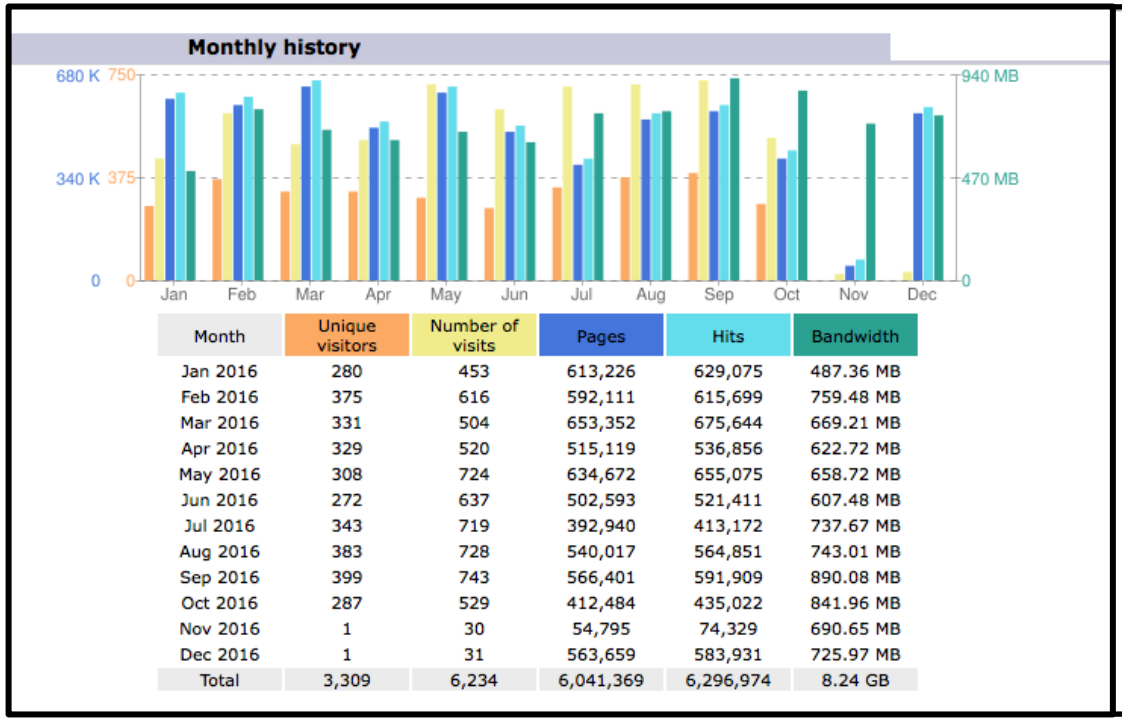


Current caNanoLab Content:

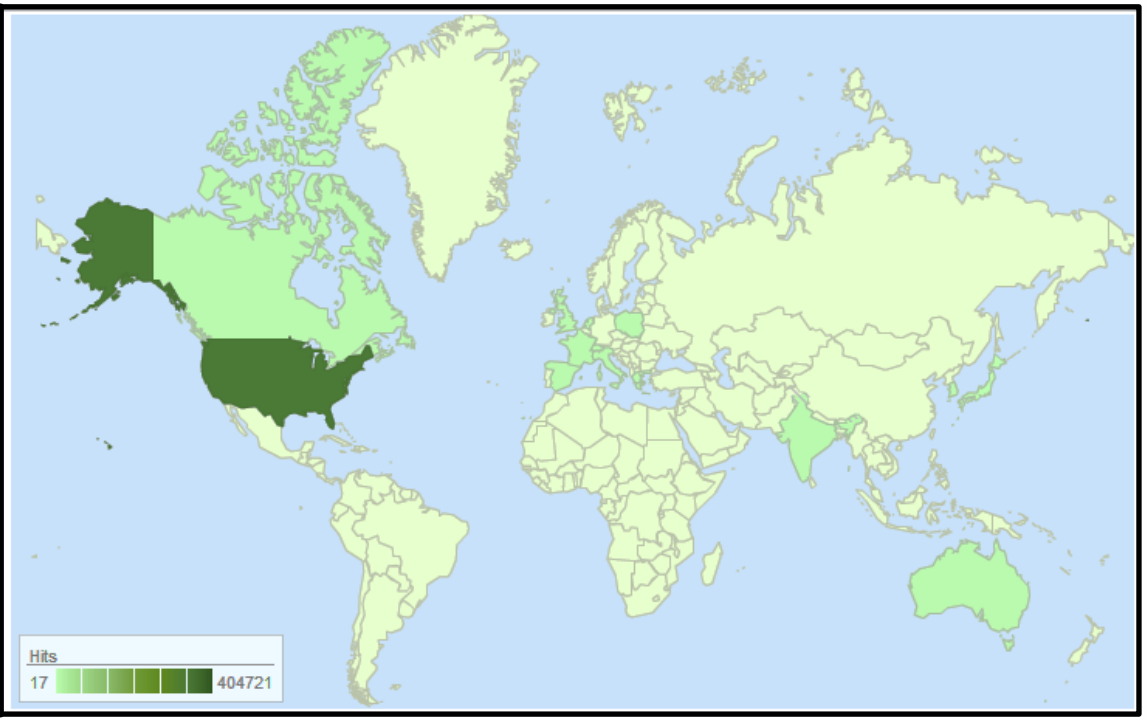
- **1,217 Sample Records**
  - **130 sample sources; 4,817 characterizations**
- **1,925 Publications**
- **50 Protocols**
- **Particle types include: liposomes, metal, metal oxide, silica, polymers, emulsions, dendrimers, and more**

- In-house curator; submission directly by users encouraged!
- Initial data sources Alliance and NCL; sources have grown to include laboratories across the U.S. and other countries; ~10% derived from international publications (e.g., United Kingdom, Canada, China, Greece)
- Researchers can submit data via web-based forms and download reports in a spreadsheet-based format
- Search for samples, publications, and protocols by a variety of factors such as keyword, name, PubMed ID/DOI (publications), characterization, and composition

caNanoLab Usage



Month	Unique visitors	Number of visits	Pages	Hits	Bandwidth
Jan 2016	280	453	613,226	629,075	487.36 MB
Feb 2016	375	616	592,111	615,699	759.48 MB
Mar 2016	331	504	653,352	675,644	669.21 MB
Apr 2016	329	520	515,119	536,856	622.72 MB
May 2016	308	724	634,672	655,075	658.72 MB
Jun 2016	272	637	502,593	521,411	607.48 MB
Jul 2016	343	719	392,940	413,172	737.67 MB
Aug 2016	383	728	540,017	564,851	743.01 MB
Sep 2016	399	743	566,401	591,909	890.08 MB
Oct 2016	287	529	412,484	435,022	841.96 MB
Nov 2016	1	30	54,795	74,329	690.65 MB
Dec 2016	1	31	563,659	583,931	725.97 MB
Total	3,309	6,234	6,041,369	6,296,974	8.24 GB



- ~4000 unique visitors for all of 2016—average 330 unique visitors/month
- Top countries accessing caNanoLab: United States, Taiwan, Germany, Japan, Great Britain, Romania, Italy, Canada, India

Screenshots

Protocol Submission

Update Protocol — Glossary

Protocol Type *	physico-chemical assay
Protocol Name*	NIST - NCL Joint Assay Protocol, PCC-13
Protocol Abbreviation	PCC-13
Protocol Version	1.1
Protocol File	○ Upload ◉ Enter File URL
	http://ncl.cancer.gov/NCL_Method_PCC-13.pdf [Disclaimer]
File Title	Measuring the pH of Nanoparticle Suspensions
Description	Protocol for measuring the pH of dilute nanoparticle suspensions of composition similar to NIST Reference Materials (RMs) 8011, 8012, and 8013, which contain gold nanoparticles in a dilute electrolyte solution

Access to the Protocol Add

Publication Submission

Update Publication

Publication Type *	peer review article
Publication Status*	published
PubMed ID	Click to look up PubMed Identifier: 20080556
	clicking outside of the text field after entering a valid PubMed ID enables auto-population of PubMed related fields
Digital Object ID	10.1073/pnas.0909565107
Title*	Cooperative nanomaterial system to sensitize, target, and treat tumors.
Journal	Proceedings of the National Academy of Sciences of the United States of America
Year of Publication	2010
Volume	107
Start Page	981
End Page	986

Authors Add

First Name	Last Name	Initials	
Ji-Ho	Park	JH	Edit
Geoffrey	Maltzahn	G	Edit
Mary	Xu	MJ	Edit
Valentina	Fogal	V	Edit
Venkata	Kotamraju	VR	Edit
Erkki	Ruoslahti	E	Edit
Sangeeta	Bhatia	SN	Edit
Michael	Sailor	MJ	Edit

Keywords *(one keyword per line)*	ANTINEOPLASTIC AGENTS/ADMINISTRATION & DOSAGE/THERAPEUTIC USE CELL LINE, TUMOR Doxorubicin/administration & dosage/therapeutic use
Description	A significant barrier to the clinical translation of systemically administered therapeutic nanoparticles is their tendency to be removed from circulation

Sample Search

SAMPLE LINKS

Search Existing Samples
Enter search criteria to obtain information on samples of interest.
Advanced Sample Search
Enter advanced search criteria based on caNanoLab metadata to obtain information on samples of interest.

Sample Search — Adv

Keywords	*searching characterization keywords, publication keywords and text in characterization descriptions enter one keyword per line*
Sample Name	contains
Sample Point of Contact	contains — *searching organization name or person name*
Nanomaterial Entity	biopolymer, carbon, carbon black, carbon nanotube
Functionalizing Entity	Magnetic Particle, Monomer, Polymer
Function	endosomolysis, imaging function, magnetic
Characterization	Character

Reset Search

Sample Characterization

Assay Type	size
Point of Contact	DNT
Design Description	The effect of size based on 25 degree Celsius and Saline solvent
Experiment Configurations	Technique: dynamic light scattering(DLS); Instruments: dynamic light scattering instrument (Malvern); Description

Characterization Results — Data and Conditions

PDI (observed)	size (Z-average,nm)	temperature (observed,Celsius)
0.235	7.4	25

Files — Statistics graph base… Celsius

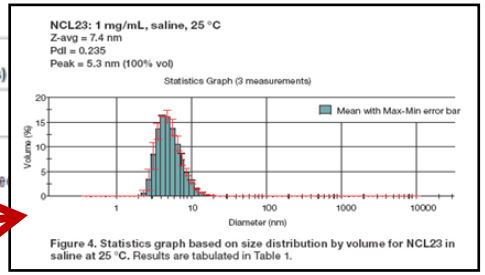


Figure 4. Statistics graph based on size distribution by volume for NCL23 in saline at 25 °C. Results are tabulated in Table 1.

Assay Type	size
Point of Contact	DNT
Design Description	The effect of size based on 25 degree Celsius and PBS solvent
Experiment	Technique; Instruments; Description

NCI Alliance for Nanotechnology in Cancer

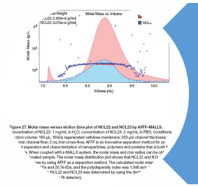
caNanoLab Data Submission

General Information

••Submit Sample Name and Investigator or other point of contact

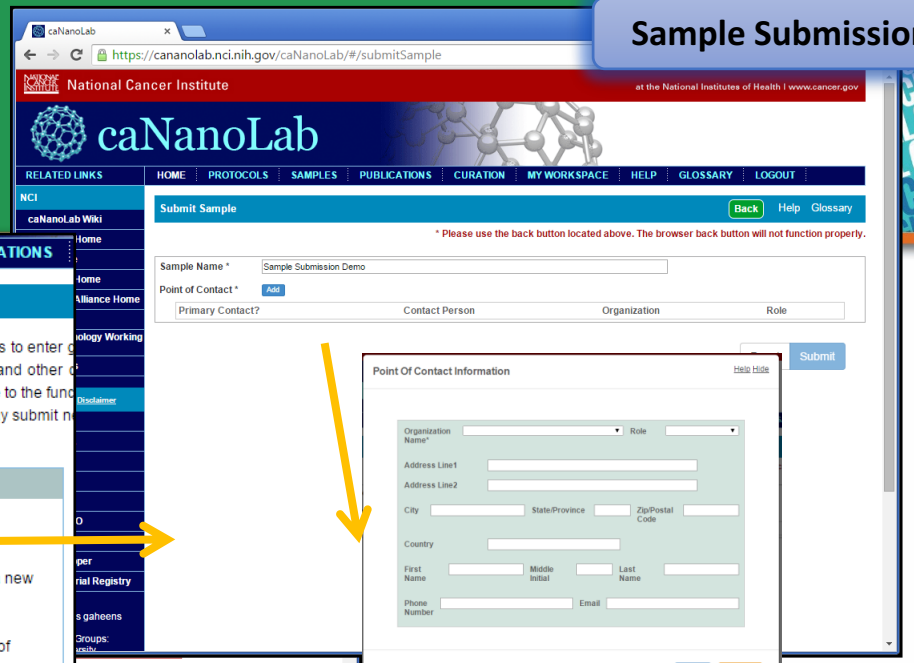
Composition

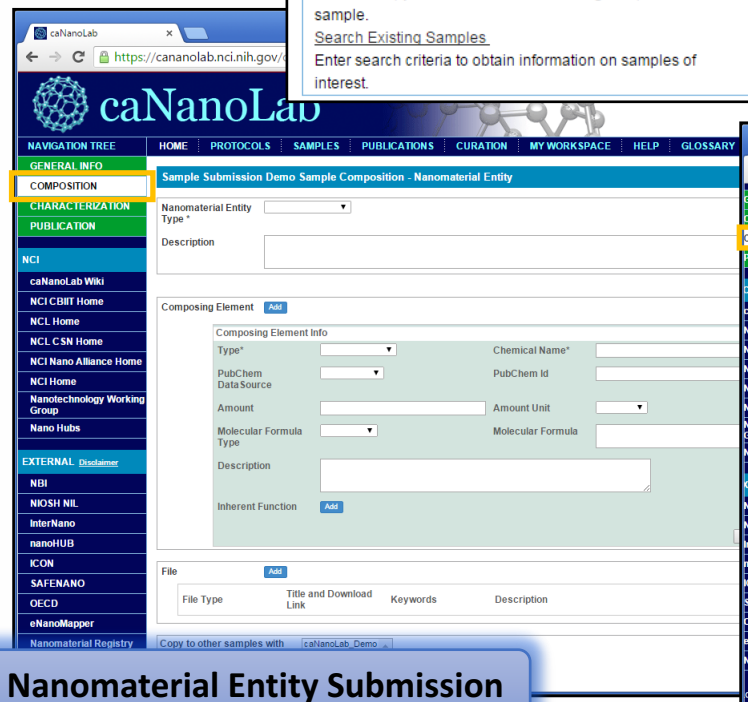
••Submit Nanomaterial and Functionalizing Entities and Chemical Associations

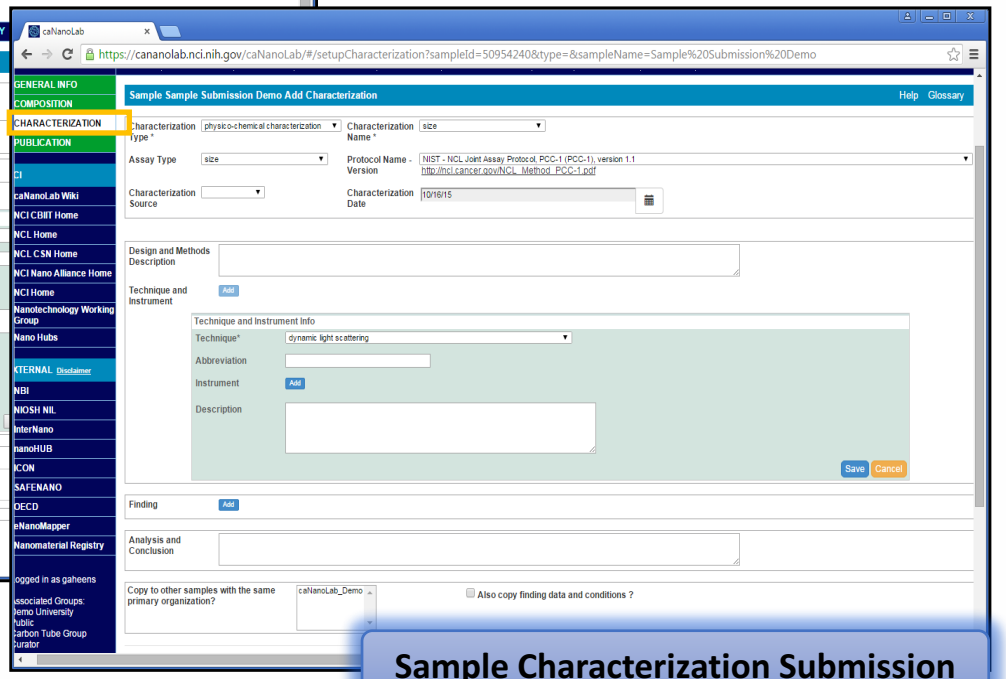


Characterizations

••Submit Physico-Chemical, *In Vitro*, and/or *In Vivo* Characterizations







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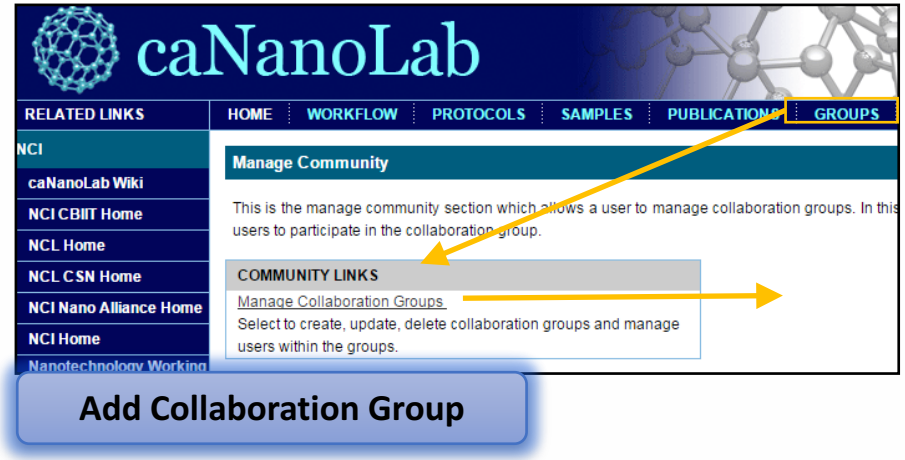
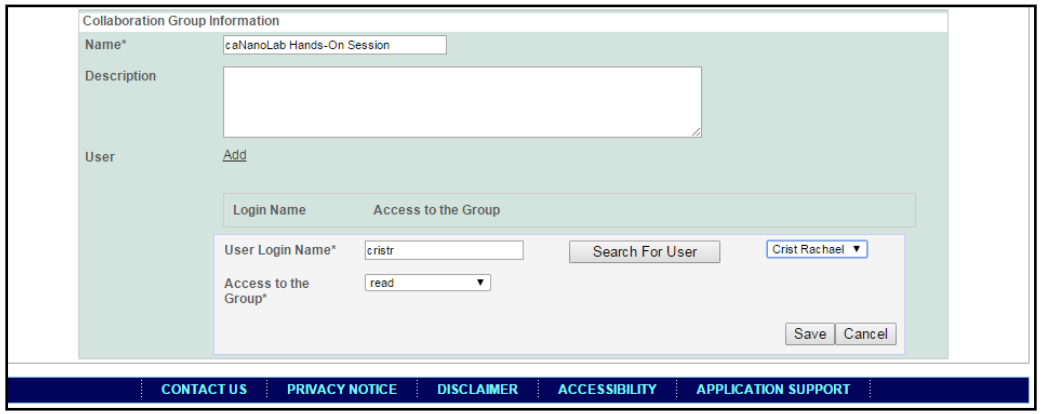
caNanoLab Data Sharing Options

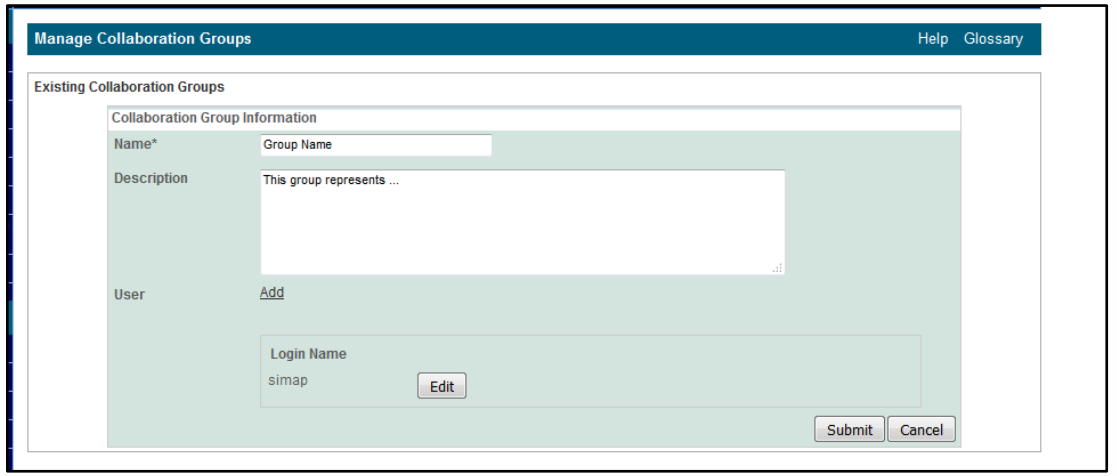
Modernized authorization (user access) modules





- Data Sharing Options: private, sharing with another caNanoLab registered user, collaboration group or request to make public.

- The Collaboration Group Feature: all group members will be added with the same access level—Read and Edit.



caNanoLab Functionality

- Usability enhancements from feedback obtained via the caNanoLab survey
- myWorkspace feature to allow users to view submitted samples, protocols, and publications and their submission status
- myFavorites feature to allow user to save samples, protocols, and publications for easy access
- Support for Advanced and Google-like Search capabilities

MyWorkspace

Samples Protocols Publications

My Samples

Actions	Sample Name	Sample Submission Status	Created Date	Sample Access
View Edit	Dendrimer-Demo	In Draft	12/17/10	(Owner, Shared by: Curator, Demo University)
View Edit	Liposome-Demo	In Draft	12/9/11	(Owner, Shared by: Curator)
View Edit	Carbon_Nanotube-Demo	In Draft	2/29/12	(Owner, Shared by: Carbon Tube Group, Curator)
View Edit	Metal_Particle-Demo	In Draft	4/24/12	(Owner, Shared by: Curator)

My Protocols

Actions	Protocol Name	Protocol Submission Status	Created Date	Protocol Access
View Edit	NIST - NCL Joint Assay Protocol, PCC-6	Retracted	12/8/10	(Owner, Shared by: Curator, Public)
View Edit	NIST - NCL Joint Assay Protocol, PCC-7	Approved	12/8/10	(Owner, Shared by: Curator, Public)
View Edit	NIST - NCL Joint Assay Protocol, PCC-10	Approved	12/8/10	(Owner, Shared by: Curator, Public)
View Edit	NIST - NCL Joint Assay Protocol, PCC-8	Approved	12/8/10	(Owner, Shared by: Curator, Public)
View Edit	NIST - NCL Joint Assay Protocol, PCC-9	Approved	12/8/10	(Owner, Shared by: Curator, Public)
View Edit	NIST - NCL Joint Assay Protocol, PCC-11	Retracted	12/8/10	(Owner, Shared by: Curator, Public)
View Edit	NIST - NCL Joint Assay Protocol, PCC-14	Approved	12/8/10	(Owner, Shared by: Curator, Public)
View Edit	NIST - NCL Joint Assay Protocol, PCC-12	Approved	12/8/10	(Owner, Shared by: Curator, Public)
View Edit	NIST - NCL Joint Assay Protocol, PCC-13	Approved	12/8/10	(Owner, Shared by: Curator, Public)
View Edit	ITA-14	Approved	12/8/10	(Owner, Shared by: Curator, Public)
View Edit	ITA-5.1	Approved	12/8/10	(Owner, Shared by: Curator, Public)
View Edit	ITA 5.2	Approved	12/8/10	(Owner, Shared by: Curator, Public)
View Edit	NCL Method GTA-14	Approved	12/8/10	(Owner, Shared by: Curator, Public)
View Edit	NCL Method GTA-11	Approved	12/8/10	(Owner, Shared by: Curator, Public)
View Edit	NCL Method GTA-12	Approved	12/8/10	(Owner, Shared by: Curator, Public)

My Publications

Advanced Search

Advanced Sample Search

Sample Criteria

-- Please Select -- | -- Please Select -- | Add | Reset

Composition Criteria

nanomaterial entity dendrimer Edit

-- Please Select -- | -- Please Select -- | with chemical name | -- Please Select -- | Add | Reset

Characterization Criteria

physico-chemical characterization	size	size	>	10	nm	Edit
in vitro characterization	cytotoxicity	LC50	>	10	mg/L	Edit

-- Please Select -- | -- Please Select -- | -- Please Select -- | Add | Reset

AND OR

AND OR

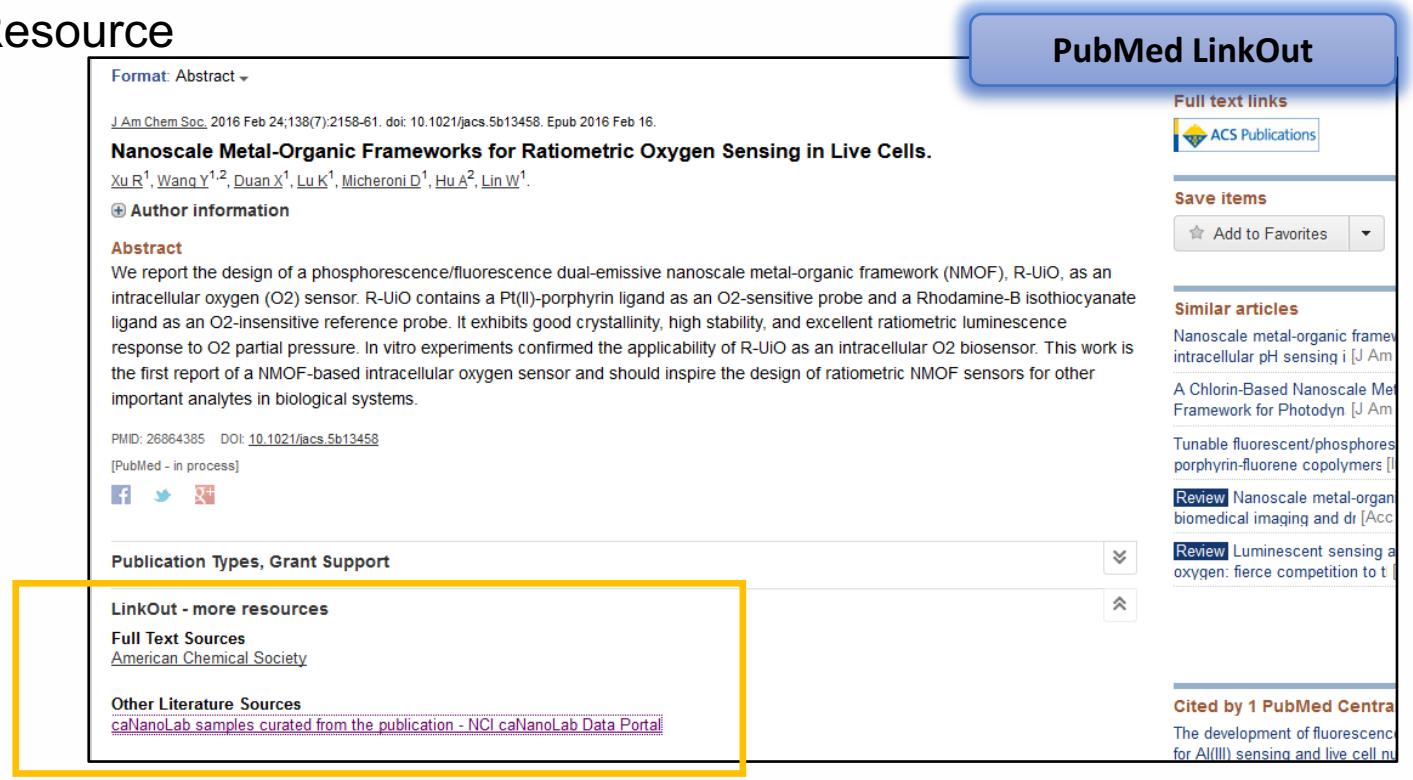
Searching without any parameters returns all samples.

Reset Search

Promoting caNanoLab Data

NIH and NCI

- Both caNanoLab and Nanomaterial Registry on list of NIH Data Sharing Repositories maintained by National Library of Medicine.
- NCI Data Catalog lists caNanoLab—list of data collections produced by NCI initiatives
- PubMed LinkOut Resource

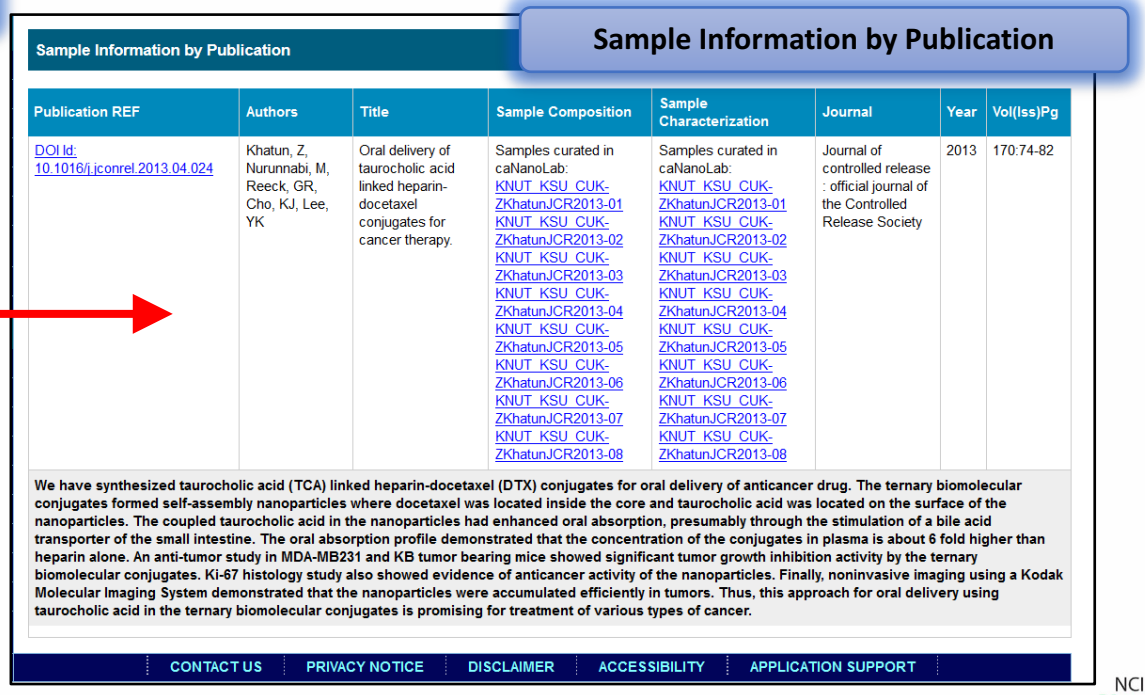


https://www.ncbi.nlm.nih.gov/pubmed/?term=loprovncicananolab[SB]

Promoting caNanoLab Data

Publishers and Journals

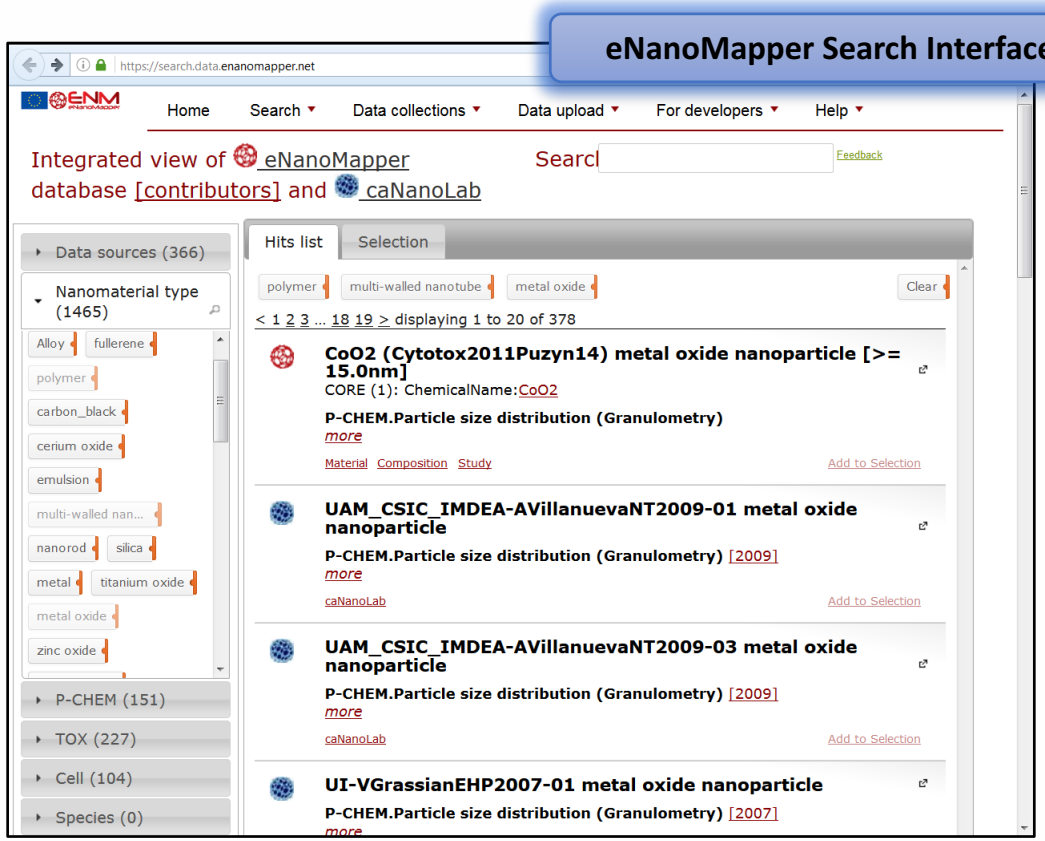
- Nature, PLOS, and Elsevier journals added nanomaterial databases as recommended data repositories
  - Opportunities to publish data descriptor articles with Nature's *Scientific Data*
  - Have an established bidirectional interface with Elsevier articles and caNanoLab data



Promoting caNanoLab Data

Integrating with other Databases

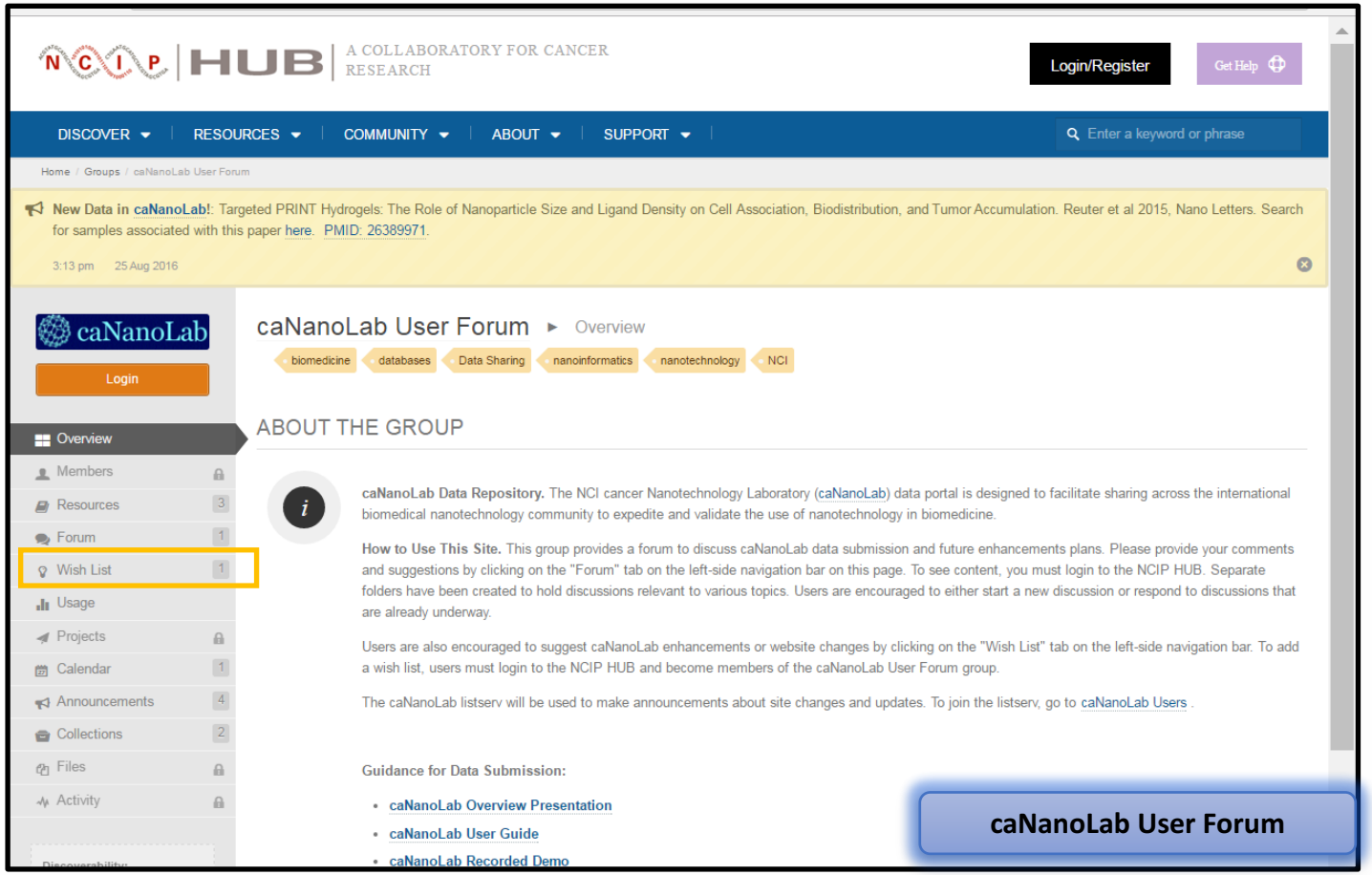
- Nanomaterial Registry
- eNanoMapper –European project focused on the development of a computational infrastructure for engineered nanomaterial toxicological data management



https://search.data.enanomapper.net/

caNanoLab User Forum

- Forum for users to discuss caNanoLab and data sharing
- Provides guidance for data submission
- Submit New Feature Request or defect using Wish List tab



https://nciphub.org/groups/cananolab_usability/

Upcoming/Ongoing Activities

- Release of caNanoLab 2.4 in August 2017
  - Follow-up with data coordinators
- Accessing image data through caNanoLab
  - Extension of The Cancer Imaging Archive (TCIA) to support preclinical images and data (Wash U CCNE)
- Development of an electronic nanomaterial data notebook
  - For collection of data while generating, sharing between laboratories, and integrating with databases (UNC-Chapel Hill CCNE)
- Acquiring data directly from users
- Increased interaction with community, publishers, and journals in support of data acquisition, and the development of guidelines that promote data sharing and data standards adoption

caNanoLab Team

- **Stephanie Morris**, Project Lead, Office of Cancer Nanotechnology Research
- **Mervi Heiskanen**, Project Lead, Center for Biomedical Informatics and Information Technology
- **Michal Lijowski**, Data Curator
- **Philippa Barnes**, Project Manager

Support Slides

Data Curation Procedures

Publication Identification

NCI caNanoLab team identifies publications based on curation criteria

Data Extraction

Curator extracts data from publica-tion

caNanoLab

caNanoLab Submission

Curator submits data into caNano-Lab

Author Notification

NCI Nano Alliance requests additional information from author

Data Publication

Curator enables public view of data

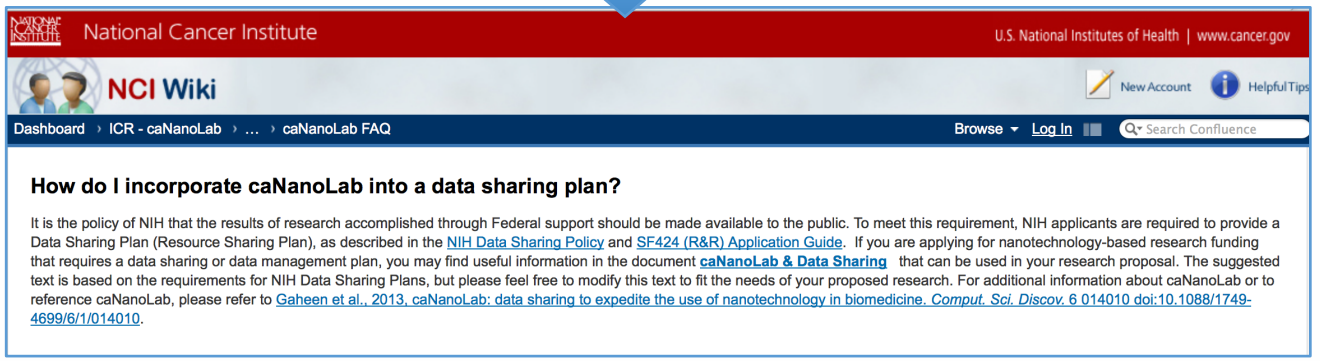
Encouragement to Requirement: Nanomaterials Data Deposition

- For Phase III Alliance, **nanomaterial data deposition a Term and Condition of Award**
  - Included in funding opportunity announcements
- caNanoLab inclusion in data sharing plan; and the designation of at least one scientifically qualified person as nanomaterial data sharing coordinator required once an award has been made
- Dedicated user forum to provide guidance, submit new features request, report defects

HOW TO

- How do I submit data into caNanoLab?
- How do I incorporate caNanoLab into a data sharing plan?
- How do I find nanotechnology protocols?
- How do I find Nanotechnology publications?
- How can I search for nanomaterials?
- How can I search for nanomaterial characterizations?
- Where can I get definitions for nanotechnology concepts?

https://wiki.nci.nih.gov/display/caNanoLab/caNanoLab+FAQ



Example Particle-Specific Composition Metadata

Particle Type	Metadata	# of Particles in caNanoLab
Biopolymer	Name, Type (e.g. DNA, Peptide, RNA), Sequence	62
Carbon Nanotube	Average Length, Chirality, Diameter, Wall Type (e.g. DWNT, MWNT, SWNT)	50
Dendrimer	Branch, Generation	75
Emulsion	Is Polymerized, Polymer Name	88
Fullerene	Average Diameter, Number of Carbons	16
Liposome	Is Polymerized, Polymer Name	37
Metal Oxide	Composing Elements	200
Metal Particle	Composing Elements	142
Polymer	Initiator, Is Cross Linked, Cross Link Degree	231
Quantum Dot	Composing Elements	73
Silica	Composing Elements	55
…	…	

Fall 2015

Example Characterization Assay Metadata (1 of 2)

Characterization Type	Metadata
Physico-Chemical	• **Molecular Weight** • **Physical State** (*Type=Solid-Powder…*) • **Relaxivity** (*R1, T1, R2, T2*) • **Shape** (*Type=2D-Circle…)* • **Size** (*Aspect Ratio, Diameter [Avg, Min, Max], Intensity, Size [Avg, Min, Max], Volume, PDI*) • **Solubility** (Solvent, Critical Concentration, Is Soluble) • **Surface** (isHydrophobic) • **Zeta Potential**
In Vitro	• **Blood Contact** (*Plasma Protein Binding, Hemolysis, Platelet Aggregation, Coagulation, Complement Activation*) • **Cytotoxicity** (*Cell Line, Cell Viability, IC50, Caspase 3 Apoptosis, Proliferation, Mitochondrial Membrane Potential, Mitochondrial Function, Gene Expression*) • **Enzyme Induction** (*Enzyme Name, Enzyme Induction/Suppress*ion) • **Immune Cell Function** (*CFU-GM, Leukocyte Proliferation, Phagocytosis, Cytokine Induction, Chemotaxis, Oxidative Burst, Cytotoxic Activity of NK Cells*) • **Metabolic Stability** • **Oxidative Stress** (*SH Homeostasis, Lipid Peroxidation, ROS Generation*) • **Sterility** (*Endotoxin, Bacterial/Yeast/Mold, Mycoplasma*) • **Targeting** (*Cell Binding/Internalization, Gene Expression*) • **Transfection** (*Cell Line*)

Example Characterization Assay Metadata (2 of 2)

Characterization Type	Metadata
In Vivo	• **Pharmacokinetics** *(AUC, Clearance, Clearance at Time O, Clearance Route, Clearance Timepoint, cMax, Elimination Rate Constant, Elimination Half Life, Elimination Rate, Half Life, tMax, Volume of Distribution*) • **Toxicology** (*Histopathology Finding, Organ/Tissue, Lesion Type, Clinical Observation, Organ Weight Measurement, Body Weight Measurement, Toxicology Measurement [ED50, ID50, LC50, LD50, TD50], Survival Time, Developmental Toxicology, Behavior Toxicology*) • **Imaging** (*Type, Image, Region of Interest, Image Contrast Agent Name, Image Contrast Agent Localization, Calibration Protocol*)
Ex Vivo	• **Histology** *(Organ/Tissue, Sample Preparation Protocol)* • **Imaging** *(Organ/Tissue, Cell Viability)*