



**caBIG™**  
cancer Biomedical  
Informatics Grid™

# caNanoLab Overview

*Nanoinformatics 2010*

November 2010





**To provide nanotechnology resources to facilitate data sharing in the research community to expedite and validate the use of nanomaterials in biomedicine**

# Example Nanotechnology User Scenario



An existing drug used to target cancer causes significant side effects. Can nanomaterial-assisted targeted delivery increase efficacy and reduce side effects?

- **Identify and synthesize a nanomaterial delivery system that:**
  - Is biocompatible and has a long half-life
  - Is designed to effectively target the cancer cells
  - Is multi-functional (imaging, therapeutic, targeting agents on the same vehicle)
- **Perform physico-chemical characterizations (size, zeta potential) to validate nanomaterial synthesis and determine the stability of the particle**
- **Perform *in vitro* characterizations (cytotoxicity, immune cell function) to determine the toxicity and effectiveness of the nanomaterial formulation in model cell lines. Compare the nanomaterial delivery system to the drug alone and the nanomaterial alone.**
- **Perform *in vivo* characterizations (pharmacokinetics, toxicology) on established animal tumor models. Efficacy, dosing, and side effects of the current drug dosing protocol are compared with the targeted nanomaterial delivery system.**

# caNanoLab Overview



- 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, physico-chemical and *in vitro* characterizations (*in vivo* coming soon), protocols, and publications
- caNanoLab leverages and extends concepts from the NCI's Enterprise Vocabulary Services (EVS) and the NanoParticle Ontology (NPO)
- caNanoLab is engineered to enable data sharing in a semantically interoperable fashion in the spirit of the NCI cancer Biomedical Informatics Grid (caBIG<sup>®</sup>) program

caNanoLab Home - Microsoft Internet Explorer

Address: <http://cananolab.nci.nih.gov/cananolab/welcome.do>

National Cancer Institute U.S. National Institutes of Health | www.cancer.gov

## caNanoLab

QUICK LINKS: NCI, caNanoLab Wiki, NCI CBIT Home, NCL Home, NCL CSN Home, NCI Nano Alliance Home, NCI Home

EXTERNAL: NBI, NIOSH NCL, InterNano, nanoHUB, ICON, SAFEMANO

Visitor Count: 44406 Since 09/03/2010

HELP GLOSSARY

Welcome to caNanoLab

Welcome to the cancer Nanotechnology Laboratory (caNanoLab) portal. caNanoLab is a data sharing portal designed to facilitate information sharing in the biomedical nanotechnology research community to expedite and validate the use of nanotechnology in biomedicine. caNanoLab provides support for the annotation of nanomaterials with characterizations resulting from physico-chemical and *in vitro* assays and the sharing of these characterizations and associated nanotechnology protocols in a secure fashion.

Browse caNanoLab

Data Type	Public Results
<b>Search Protocols</b> Search for nanotechnology protocols leveraged in performing nanomaterial characterization assays.	26 Protocols
<b>Search Samples</b> Search for information on nanomaterials including the composition of the nanomaterial, results of physico-chemical, <i>in vitro</i> , and other characterizations, and associated publications. See also <a href="#">Advanced Sample Search</a>	634 Samples <a href="#">More State</a>
<b>Search Publications</b> Search for information on nanotechnology publications including peer reviewed articles, reviews, and other types of reports related to the use of nanotechnology in biomedicine.	1070 Publications

Primary caNanoLab features include:

- Secure submission of protocols, samples (nanomaterials), and publications
- Basic search facilities for searching for protocols, samples, and publications
- Advanced search facilities for formulating range or nested queries
- Tools for managing users via NCI Common Security Module (CSM)
- Data services available through the caBIG<sup>®</sup> grid (c)

HOW TO

Below are frequently asked questions on caNanoLab:

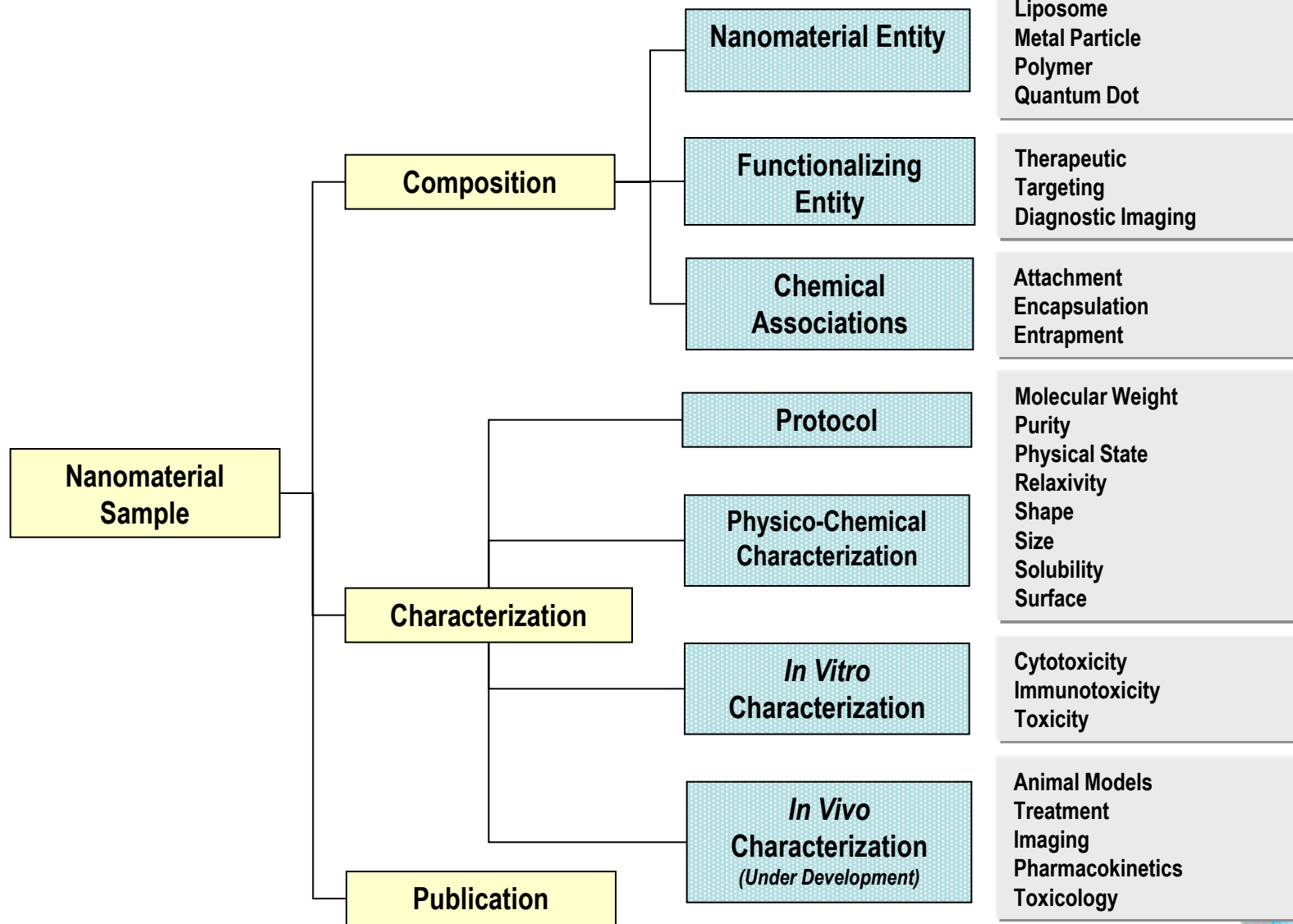
Functional

- How do I find nanotechnology protocols?
- How do I find Nanotechnology publications?
- How can I search for nanomaterials?
- How can I search for nanomaterial characterization?
- Where can I get definitions for nanotechnology?

Current Version: caNanoLab 1.5.1

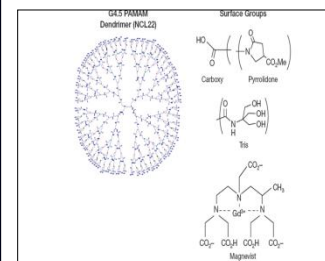
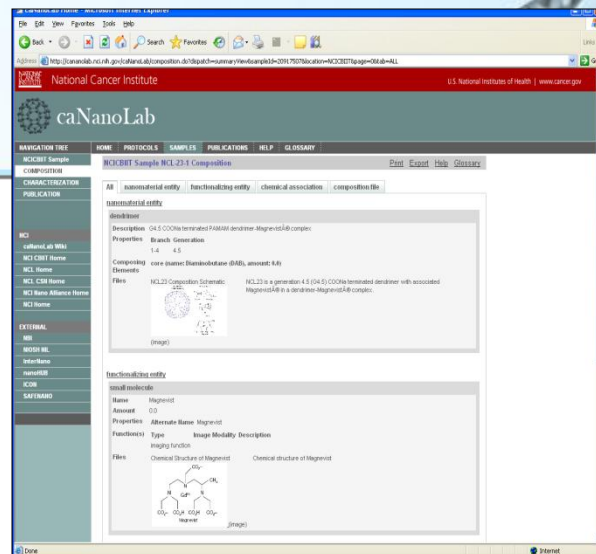
<http://cananolab.nci.nih.gov>

# caNanoLab High-Level Concepts

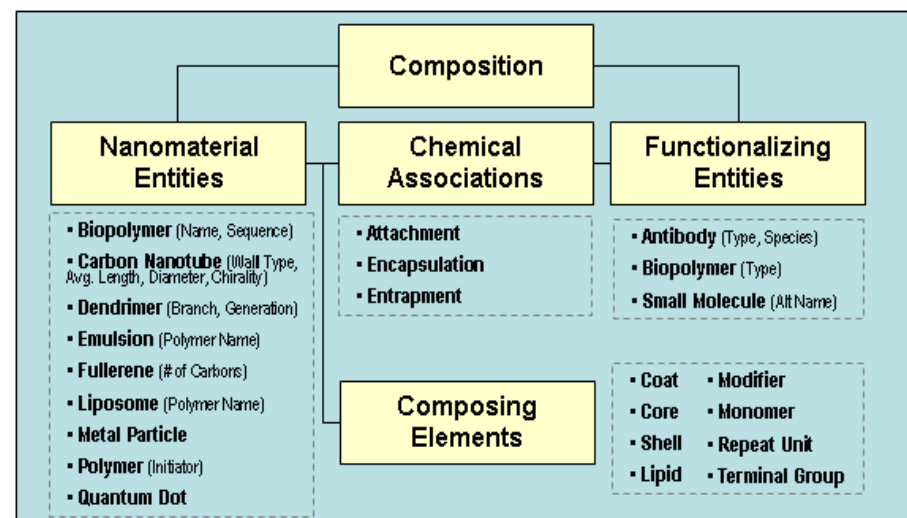


# Composition

- **Composition information includes: nanomaterial entities, functionalizing entities, and chemical associations**
- **A nanomaterial entity is the base nanomaterial (e.g. dendrimer) and composing elements (e.g. core)**
- **Nanomaterial entity types (e.g. dendrimer) have different composition properties (e.g. branch, generation)**
- **Functionalizing entities give the material the intended application (e.g. small molecule)**
- **Chemical associations represent the linkage and bond types between material components**
- **Supports the formulation of complex nanomaterials (e.g. liposome encapsulated in a quantum dot)**



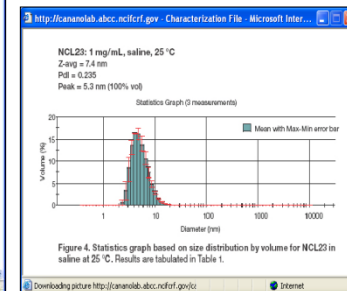
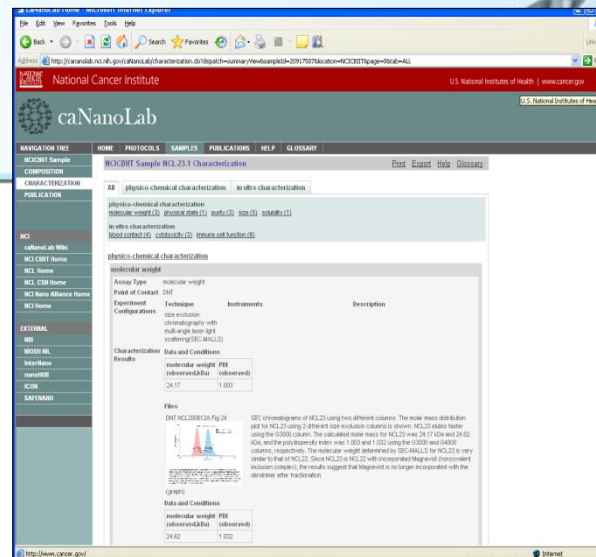
## Dendrimer Composition



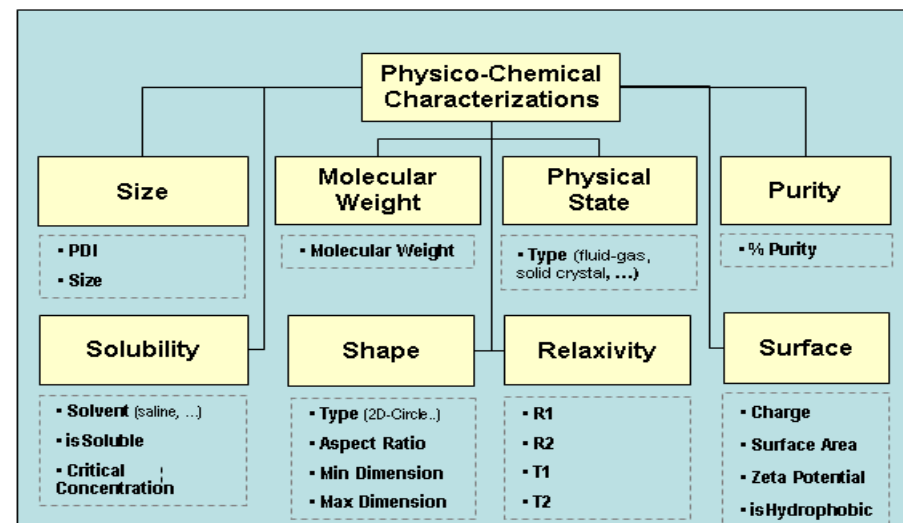
## caNanoLab Composition Concepts

# Characterizations: Physico-Chemical

- Physico-Chemical Characterizations describe the material and structural properties of a nanomaterial
- Nanomaterials are polydisperse and exhibit diverse physico-chemical properties based on experimental conditions (e.g. pH, temperature, solvent) or applied instruments/techniques (e.g. Dynamic Light Scattering)
- Physico-Chemical Characterizations (e.g. size, shape) have a direct impact on biological interactions



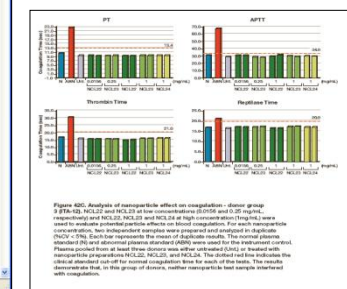
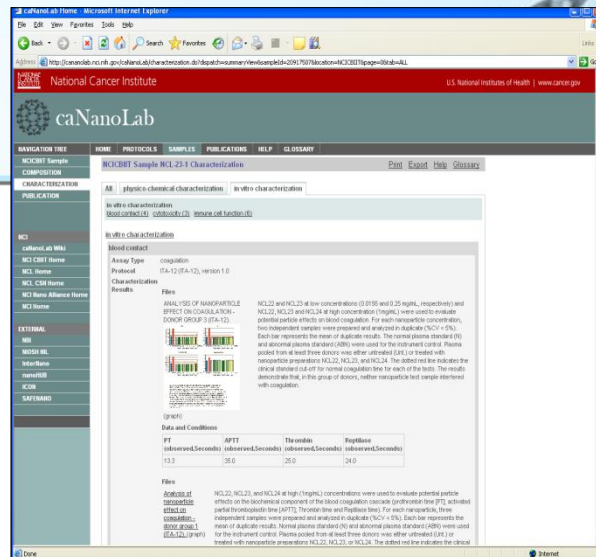
## Molecular Weight



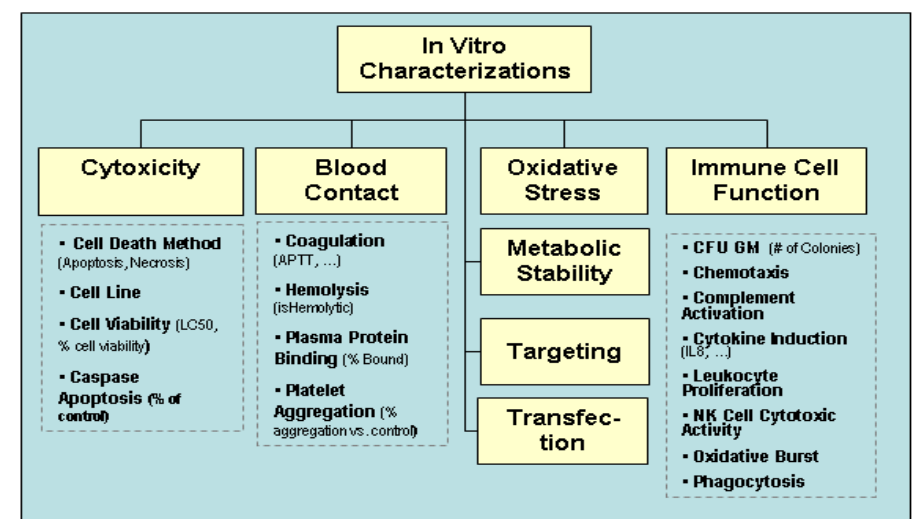
## caNanoLab Physico-Chemical Characterization Concepts

# Characterizations: In Vitro

- **In Vitro** Characterizations determine the effect of nanomaterials on cultured cells or tissues
- **In Vitro** Characterizations test a nanomaterial's binding, pharmacology, and other properties monitored by cellular and molecular biology methods
- **In Vitro** Characterizations also determine a nanomaterial's blood contact properties, interactions with cellular-level components, and therapeutic and/or diagnostic functionality



## Coagulation

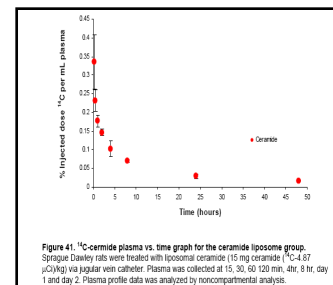


## caNanoLab In Vitro Characterization Concepts

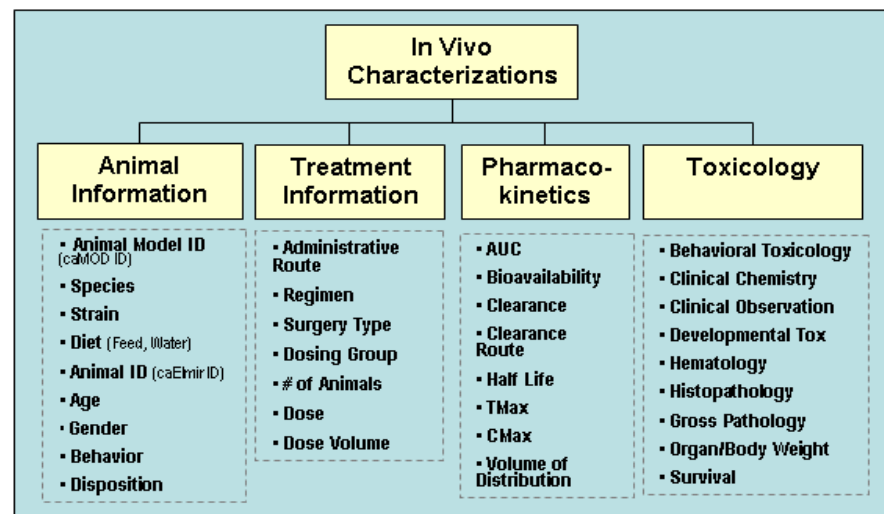


# Characterizations: *In Vivo* (Coming Soon)

- *In Vivo* Characterizations determine the effect of the nanomaterial on living organisms
- *In Vivo* Characterizations include animal information, treatment information, pharmacokinetics, and toxicology and are not specific to nanomaterials
- *In Vivo* Characterization concepts are derived from the CDISC SEND (v2.3) and SDTM (v3.2.1) standards for animal tox studies and human clinical trials pharmacokinetics, respectively
- Support for *In Vivo* Characterizations will include interfaces to NBIA (Images) and caMOD (Animal Models)



## Pharmacokinetics



caNanoLab *In Vivo*  
Characterization Concepts

# Publications

- caNanoLab allows users to search and submit Publications and other types of Reports
- Samples can be associated with multiple Publications but can be submitted without Samples
- Auto-completion has been implemented for PubMed articles leveraging PubMed's HTTP API for retrieving publication information in XML format
- caNanoLab provides access to 1000+ abstracts published by the NCI's Nanotechnology Alliance

The screenshot shows the caNanoLab search interface. The top navigation bar includes 'HOME', 'PROTOCOLS', 'SAMPLES', 'PUBLICATIONS', 'HELP', and 'GLOSSARY'. The search form is titled 'Search Publications' and includes the following fields and options:

- Publication Type:** A dropdown menu.
- Research Category:** Radio buttons for 'animal', 'cell line', 'characterization', 'clinical trials', 'in vitro', 'in vivo', and 'synthesis'.
- PubMed ID:** A text input field with an 'exact match' checkbox.
- Digital Object ID:** A text input field with an 'exact match' checkbox.
- Publication Title:** A text input field with a 'contains' dropdown menu.
- Authors:** A text input field with a 'enter one author per line' instruction.
- Keywords:** A text input field with a 'enter one keyword per line' instruction.
- Sample Name:** A text input field with an 'exact match' checkbox.
- Composition:** A dropdown menu with options: 'biopolymer', 'carbon black particle', 'carbon nanotube', and 'carbon particle'.
- Material Entry:** A dropdown menu with options: 'Magnetic Particle Monomer' and 'Polymer'.
- Functionalizing Entry:** A dropdown menu.
- Function:** A dropdown menu with options: 'imaging function', 'other', and 'targeting function'.

At the bottom of the search form, there is a message: 'Searching without any parameters would return all publications.' and buttons for 'Reset' and 'Search'.

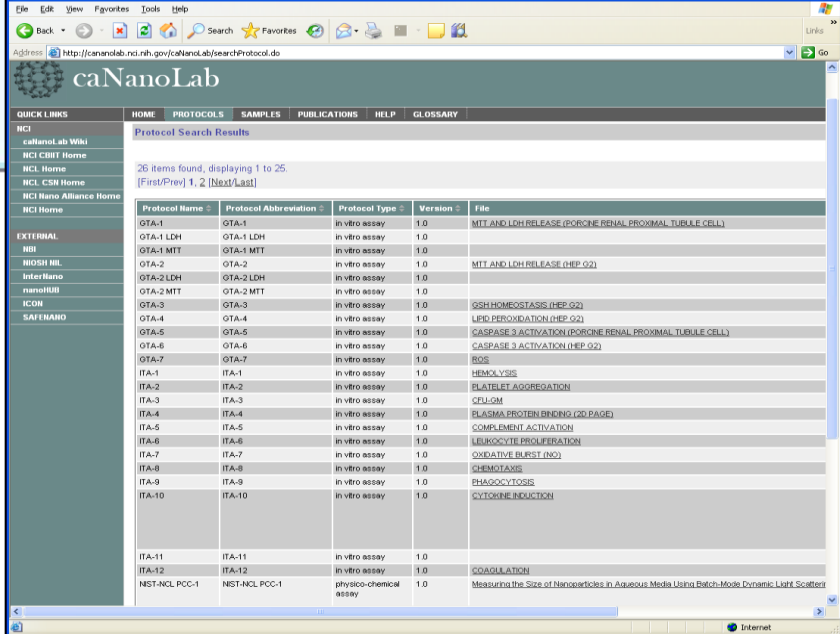
## Publication Search

The screenshot shows the caNanoLab search results page. The top navigation bar is the same as in the search form. The page is titled 'Publication Search Results' and shows '1,087 items found, displaying 1 to 25'. Below the search results, there is a table with the following columns: 'Bibliography Info', 'Publication Type', 'Research Category', 'Associated Sample Names', 'Description', 'Created Date', 'Publication Status', and 'Location'.

Bibliography Info	Publication Type	Research Category	Associated Sample Names	Description	Created Date	Publication Status	Location
DEBIRITIC NANOTECHNOLOGIES 12006. [2006] pdf.	report		NCL-20-1 NCL-21-1 NCL-22-1 NCL-23-1 NCL-24-1 NCL-25-1 NCL-26-1	Ystaz	12-20-2006	published	NCCIBT
NCL200710A FUNCTIONALIZED FULLERENES FOR CSXTY INC. NCL200710A Functionalized Fullerenes.pdf.	report		NCL-16 NCL-17 NCL-18 NCL-42 NCL-48	Ystaz	01-24-2008	published	NCCIBT
NCL200702A CERAMIDE LIPOSOMES FOR MARK KESTER PSU. NCL200702A Ceramic Liposomes.pdf.	report		NCL-48 NCL-48-4 NCL-49 NCL-49-2 NCL-50-1 NCL-51-3	Ystaz	01-24-2008	published	NCCIBT
Zohar, BS, Stern, ST, Kaiser, JM, Heikal, Y, Ogration, JD, Kessler, M, McNeil, SE. Rapid distribution of liposomal short-chain ceramide in vitro and in vivo. Drug metabolism and disposition: the biological fate of chemicals. 2008; 36:1709-1715. PMID: 18490336.	peer review article	animal cell line characterization in vitro in vivo	NCL-48 NCL-49	Ystaz	09-06-2008	published	NCCIBT
Chan, KC, Pati, AK, Veendra, TD, McNeil, SE, Issacs, HJ. Analysis of fullerene-based nanoparticles in serum matrix by CE Electrophoresis. 2007; 28:1518-1524. PMID: 17482487.	peer review article	characterization in vitro	NCL-19	Ystaz	09-06-2008	published	NCCIBT
Hill, JB, Dobrovolskaya, MA, Pati, AK, McNeil, SE. Characterization of nanoparticles for therapeutics. Nanomedicine (London, England). 2007; 2:100-104.	review	characterization in vitro in vivo	NCL-16 NCL-17 NCL-18 NCL-20-1	Ystaz	09-06-2008	published	NCCIBT

# Protocols

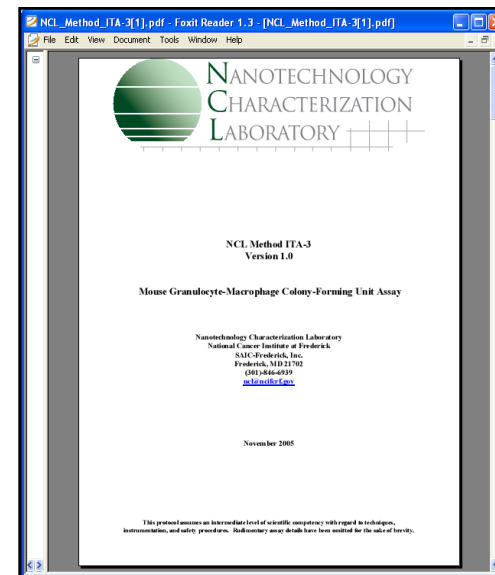
- caNanoLab allows users to submit Protocols for characterization, safety, radiolabeling, sample preparation, and other types of protocols
- Protocols can be associated with Characterizations but can be submitted without Characterizations
- Multiple versions of Protocols can be submitted
- caNanoLab provides access to protocols from the NCI Nanotechnology Characterization Laboratory (NCL)



The screenshot shows the caNanoLab website interface. The top navigation bar includes links for HOME, PROTOCOLS, SAMPLES, PUBLICATIONS, HELP, and GLOSSARY. The main content area displays 'Protocol Search Results' with 26 items found. A table lists various protocols with columns for Protocol Name, Protocol Abbreviation, Protocol Type, Version, and Title.

Protocol Name	Protocol Abbreviation	Protocol Type	Version	Title
OTA-1	OTA-1	in vitro assay	1.0	MIT AND LDH RELEASE (PORCINE RENAL PROXIMAL TUBULE CELL)
OTA-1 LDH	OTA-1 LDH	in vitro assay	1.0	
OTA-1 MIT	OTA-1 MIT	in vitro assay	1.0	
OTA-2	OTA-2	in vitro assay	1.0	MIT AND LDH RELEASE (HEP-G2)
OTA-2 LDH	OTA-2 LDH	in vitro assay	1.0	
OTA-2 MIT	OTA-2 MIT	in vitro assay	1.0	
OTA-3	OTA-3	in vitro assay	1.0	GSH HOMEOSTASIS (HEP-G2)
OTA-4	OTA-4	in vitro assay	1.0	LDH REPRODUCTION (HEP-G2)
OTA-5	OTA-5	in vitro assay	1.0	CASPASE 3 ACTIVATION (PORCINE RENAL PROXIMAL TUBULE CELL)
OTA-6	OTA-6	in vitro assay	1.0	CASPASE 3 ACTIVATION (HEP-G2)
OTA-7	OTA-7	in vitro assay	1.0	ROS
ITA-1	ITA-1	in vitro assay	1.0	HEMOLYSIS
ITA-2	ITA-2	in vitro assay	1.0	PLATELET AGGREGATION
ITA-3	ITA-3	in vitro assay	1.0	CFU-GM
ITA-4	ITA-4	in vitro assay	1.0	BUSHA PROTEIN BINDING (SD PAGE)
ITA-5	ITA-5	in vitro assay	1.0	COMPLEMENT ACTIVATION
ITA-6	ITA-6	in vitro assay	1.0	LEUKOCYTE PROLIFERATION
ITA-7	ITA-7	in vitro assay	1.0	OXIDATIVE BURST (NO)
ITA-8	ITA-8	in vitro assay	1.0	CHEMOTAXIS
ITA-9	ITA-9	in vitro assay	1.0	PHAGOCYTOSIS
ITA-10	ITA-10	in vitro assay	1.0	CYTOKINE INDUCTION
ITA-11	ITA-11	in vitro assay	1.0	
ITA-12	ITA-12	in vitro assay	1.0	COAGULATION
NST-NCL PCC-1	NST-NCL PCC-1	physico-chemical assay	1.0	Measuring the Size of Nanoparticles in Aqueous Media Using Back-Mode Dynamic Light Scattering

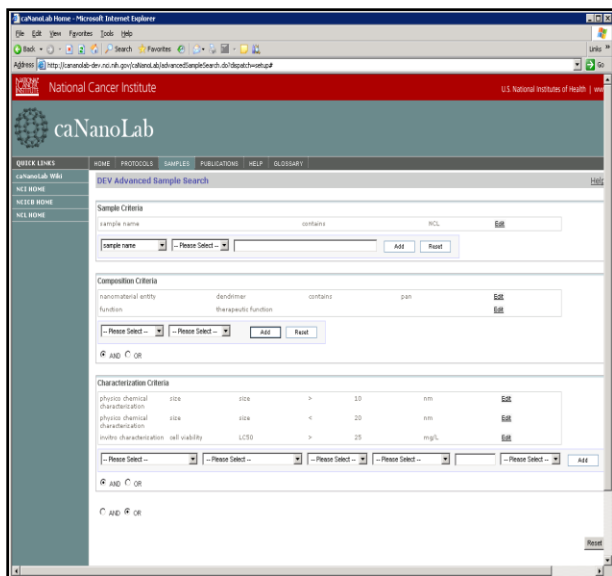
## Protocol Search Results



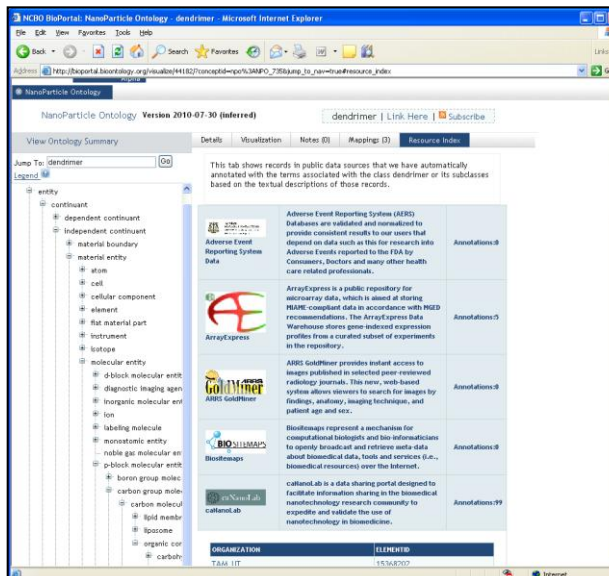
# Search Facilities



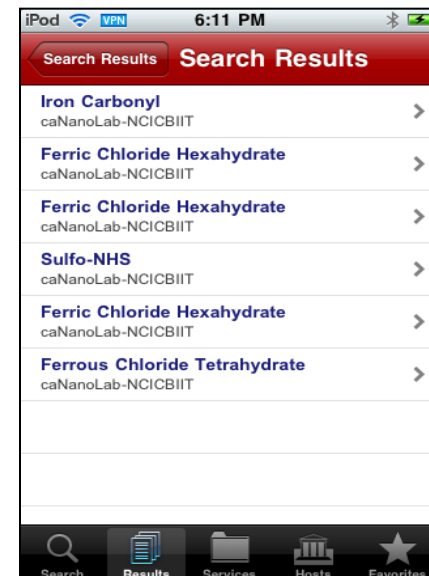
- caNanoLab provides a basic search and advanced search allowing users to perform range queries
- caNanoLab provides grid services to support access to information via server-side Application Programming Interfaces (APIs)
- The cancer Open Biomedical Resources (caOBR) ontology search facility and Grid Summary Search (GSS) iPhone App leverages caNanoLab grid services to retrieve caNanoLab data from the Nanoparticle Ontology (NPO)



Advanced Search



caOBR Ontology Search

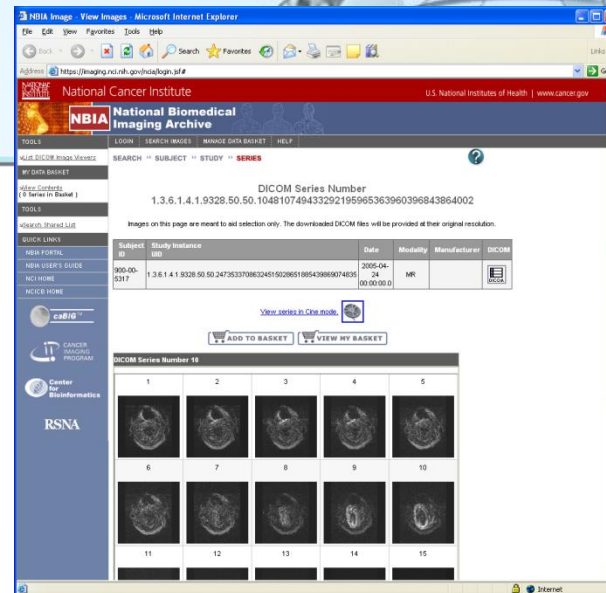


GSS iPhone App

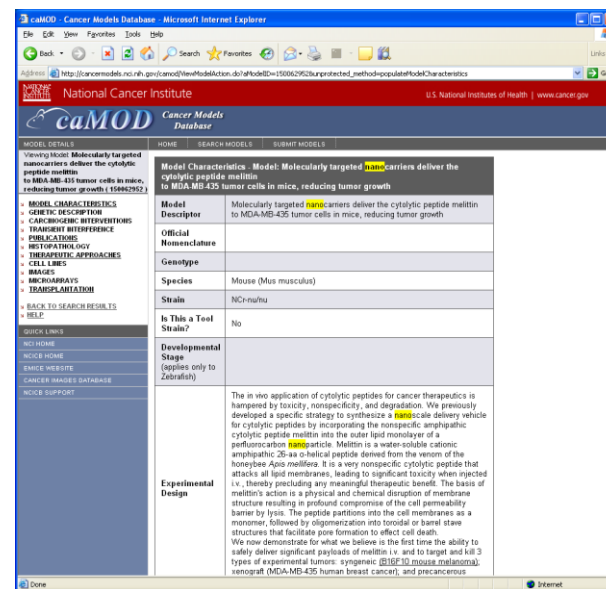


# caNanoLab Future Features

- **Support for study information and outcomes**
- **Continued support for nanotechnology standards**
  - Validate/import/export of nano-TAB
  - NCI Enterprise level services supporting nanomaterials and characterizations
- **Implementation of *in vivo* characterizations**
  - Support for pharmacokinetics and toxicology
  - Interface to the NCI's National Biomedical Imaging Archive (NBIA) for *in vivo* images
  - Interface to the NCI's cancer Model Organism Database (caMOD) for animal model information
- **Support for Structure-Activity-Relationships**
  - Interface with 3D modeling tools
- **Advanced search, visualization, and analysis**
  - Integration with GenePattern
- **Implementation of grid-level security**



National Biomedical Imaging Archive



Cancer Model Organism Database

# Acknowledgements and References



## •caNanoLab

- <http://cananolab.nci.nih.gov>

## •caNanoLab Wiki

- <https://wiki.nci.nih.gov/display/caNanoLab/caNanoLab+Wiki+Home+Page>

## •nano-TAB Project Site

- [http://gforge.nci.nih.gov/docman/index.php?group\\_id=69&selected\\_doc\\_group\\_id=5653&language\\_id=1](http://gforge.nci.nih.gov/docman/index.php?group_id=69&selected_doc_group_id=5653&language_id=1)

## •NanoParticle Ontology (NPO)

- <http://www.nano-ontology.org>
- <http://purl.bioontology.org/ontology/npo>
- <http://bioportal.bioontology.org/visualize/44737>

## •NCI Sponsor

- Piotr Grodzinski, PhD, NCI OTIR Director of Nanotechnology for Cancer Programs
- Anand Basu, NCI CBIIT Director of Applications
- Juli Klemm, PhD, NCI CBIIT ICR Director; Nano WG Sponsor
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- Dennis Thomas, PNNL
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- Marty Fritts, PhD
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- Stephen Stern, PhD