



# Community of Research: Nanotechnology Databases and Ontologies

## VISION

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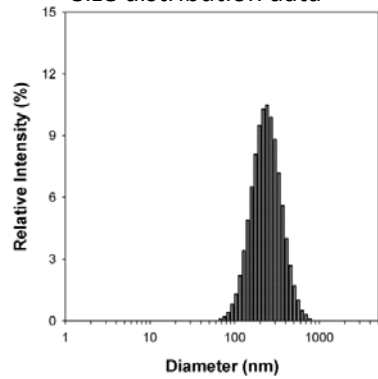


- CoR launched in May 2012  
as part of the joint EU-US initiative  
on bridging nanoEHS research efforts
- Goal: enable nanotechnology research  
through informatics

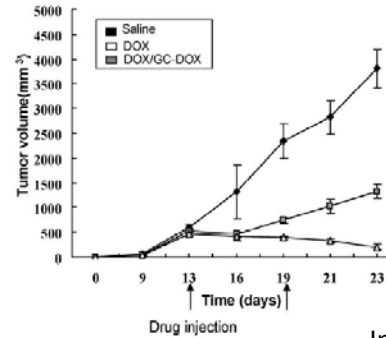
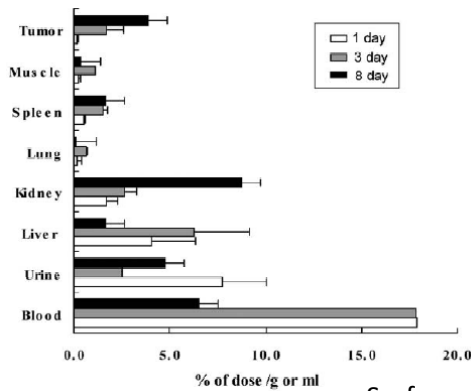


## Nanomaterials data diversity is challenging

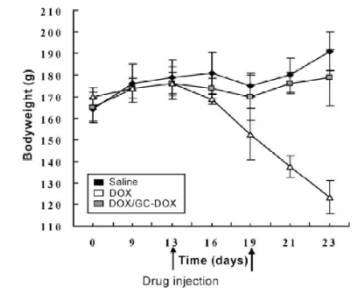
Size distribution data



Tissue biodistribution



Anti-tumor activity



Surface morphology data

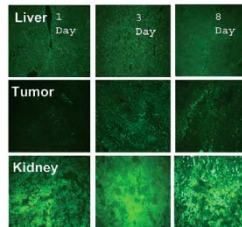
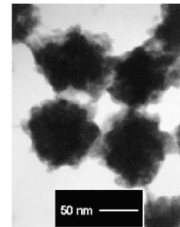
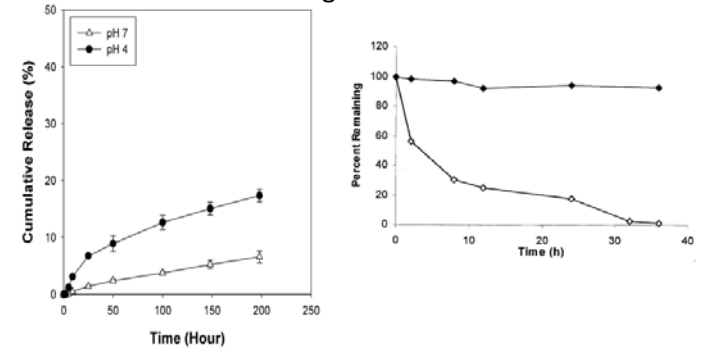


Fig. 8. Tissue accumulation of FITC-conjugated glycol-chitosan (FITC-GC) nanoaggregates for 8 days after i.v. injection in tumor-bearing mice at a dose of 10 mg/kg. Tissue accumulation measured by fluorescence microscopy.

In vitro drug release



Zeta Potential

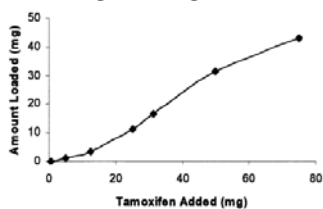
Table 1  
Zeta potential values of control and tamoxifen loaded nanoparticles<sup>a</sup>

Nanoparticle formulations	Zeta potential (mV)
Control nanoparticles	6.7 ± 1.2 <sup>b</sup>
Tamoxifen-loaded nanoparticles	25.4 ± 1.4

<sup>a</sup> Zeta potentials of the nanoparticle suspension in deionized distilled water were measured using the Brookhaven's Zeta PALS instrument.

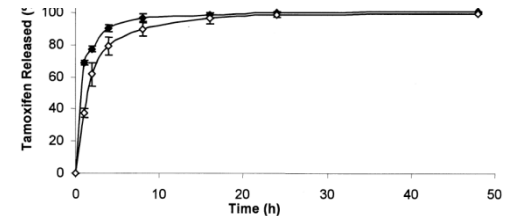
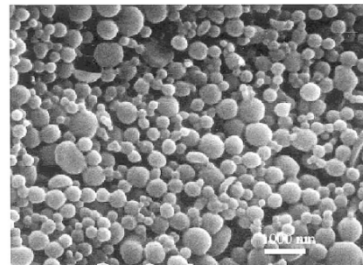
<sup>b</sup> Mean ± S.D. (n = 8).

Drug loading data



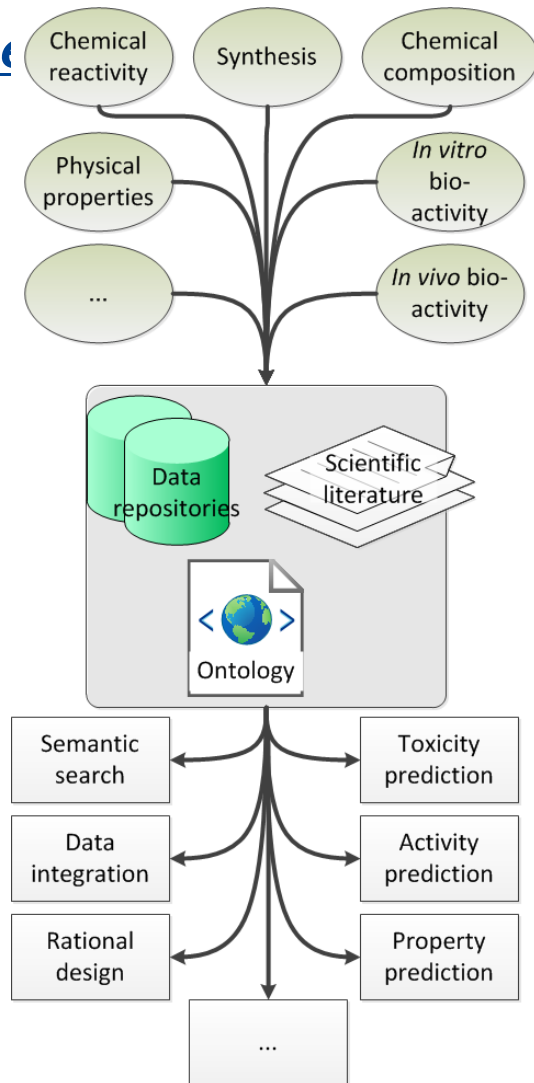
Sampling Preparation

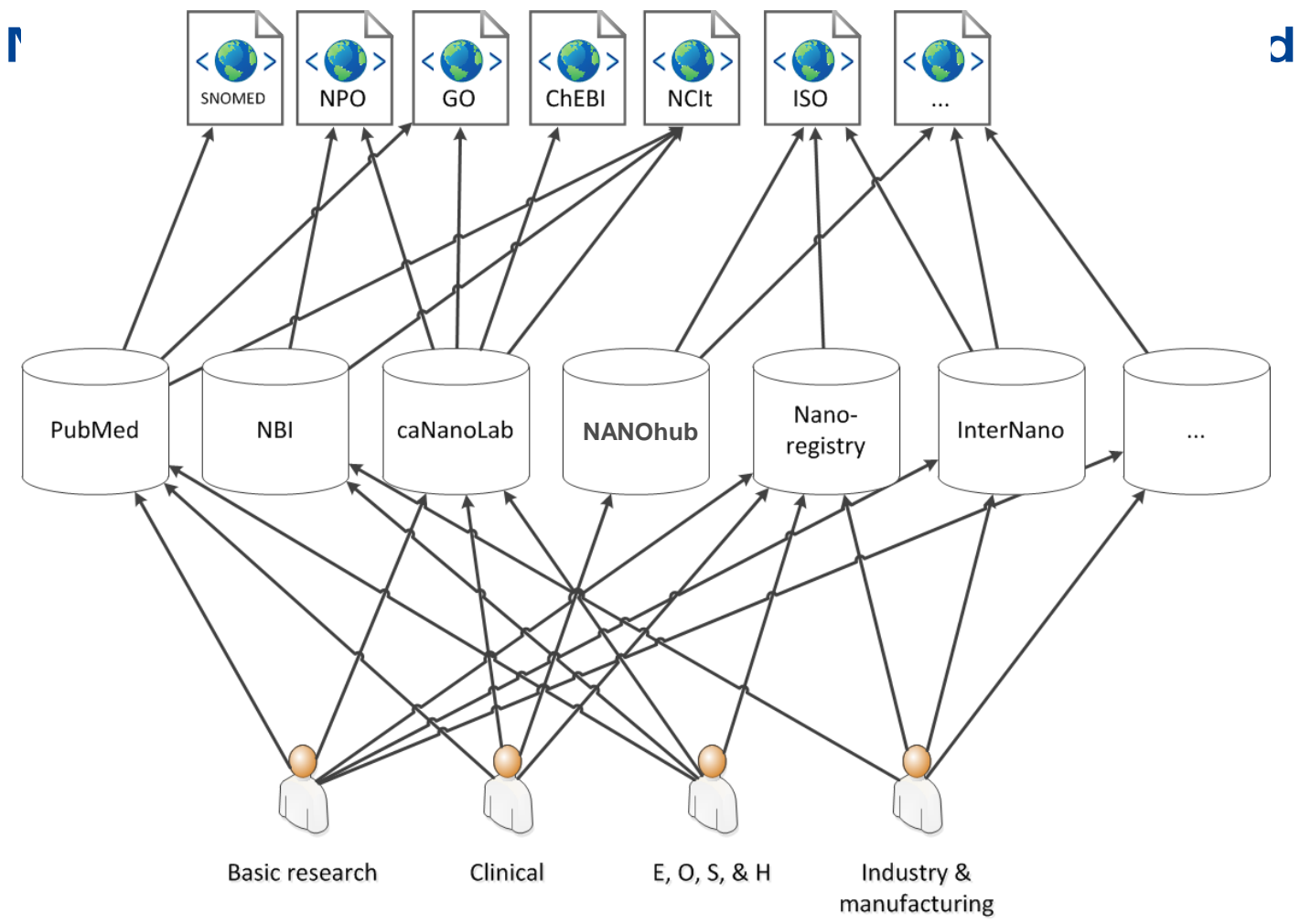
Chemical composition of nanoparticle formulation





- **Nanotechnology information** *nanotechnology information needs* systematically describe **nanomaterials** (identification, structure, morphology, composition,...)
- Nanomaterial **phys-chem properties**
- **Interaction with NM immediate environment**
- Understand **nanomaterial impact on human health**
- **Environmental** behavior
- Search for **existing data** on nanoparticle synthesis and properties
- **Exchange** nanomaterial chemical, physical, and biological **data (comparability)**
- **Design nanomaterials** with custom properties for specific applications







## Vision

### Needed

- *Interconnected, freely communicating and agreed information systems covering*
  - *nanoscale material descriptions*
  - *NM properties (intrinsic & context-dependent) and their effects,*
  - *including environmental and health-related*

### Goal

- *enable the sharing, searching, and analysis of NM characterization data across a wide range of active and archived experimental sources*
- *to give advice on how to structure these data to enable their widest possible use*

### This will

- *allow integration of pertinent risk assessment data among labs*
- *provide situational awareness of data coverage across nanomaterial categories*
- *enable predictive computational models for bridging physical properties and biological outcomes with exposure, dispersal and fate*



## Initially the CoR will focus on three areas:

- *Identification of the data elements necessary to establish common data-sharing model(s) for this domain*
- *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*

### **Vision statement:**

<http://us-eu.org/communities-of-research/search-communities-of-research/databases-ontologies/>



## Previous activities

- *Consolidated vision statement: scope, objectives*
- *2 teleconferences July & August 2012*
- *Started compilation of available resources (databases, ontology)*





Now:

- Nathan Baker (Pacific Northwest Laboratory)
- Iseult Lynch (University College Dublin)
- Breakout Discussion



## Main issues to be discussed

- Available resources and data
  - Complete inventory of resources
- Initial data sharing priorities / data needs
  - coordination with other CoRs (2-3-4)
  - Materials (description/properties)
  - Nano-bio interface
  - Health-related (hazard – exposure)
  - Environment
  - Fate....



## Main issues to be discussed

- Initial ontology concept priorities
- Workplan priorities
- Agreed future actions