

# Informatics and standards for nanotechnology

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# Outline

- ▶ **Introduction to the caBIG® Nanotechnology Working Group**
- ▶ Overview of nanotechnology informatics challenges
- ▶ Research projects
  - Ontology development
  - Data exchange standards
  - PubNano resource
  - 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
- Department of Energy
- ...

## ▶ Academia

- Washington University
- 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
- ISA-TAB community
- Oregon Nanoscience and Microtechnologies Institute
- National Nanotechnology Initiative
- National Nanomanufacturing Network
- NCI Nano Alliance



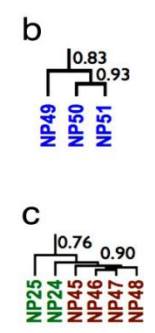
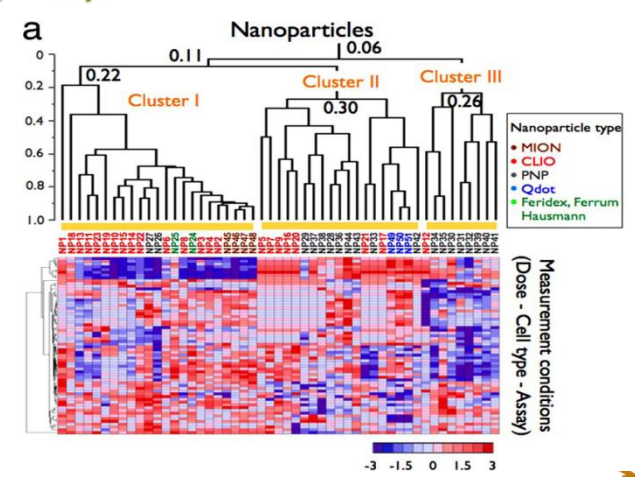
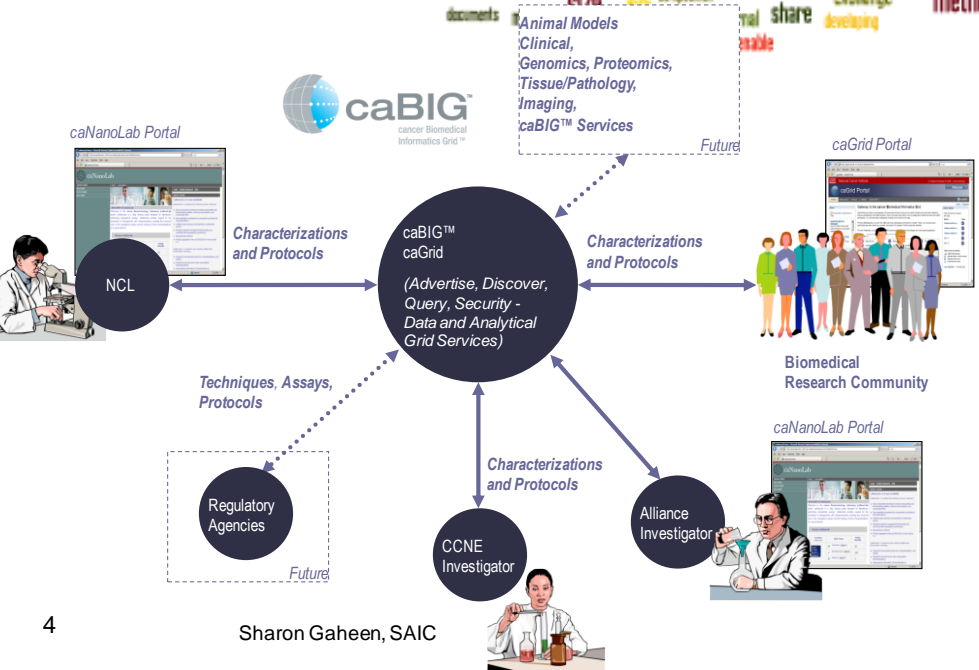
**caBIG™**  
cancer Biomedical  
Informatics Grid™



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# Working Group Scope



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



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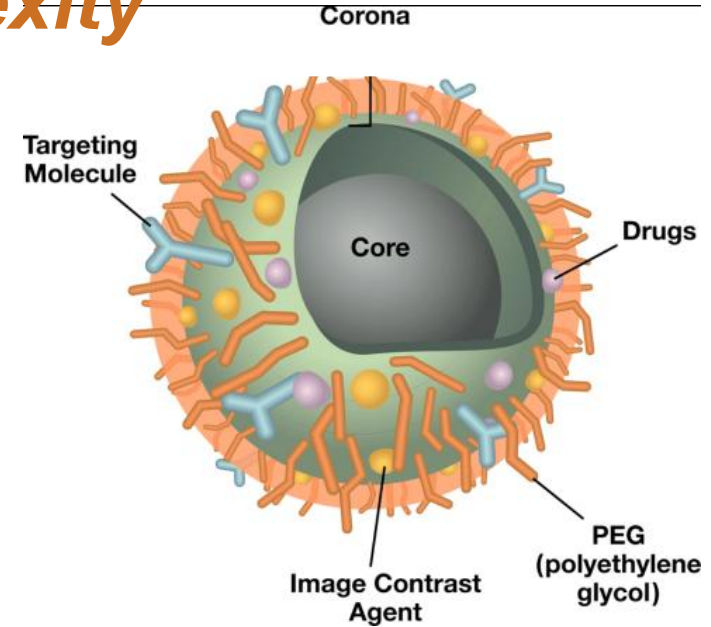


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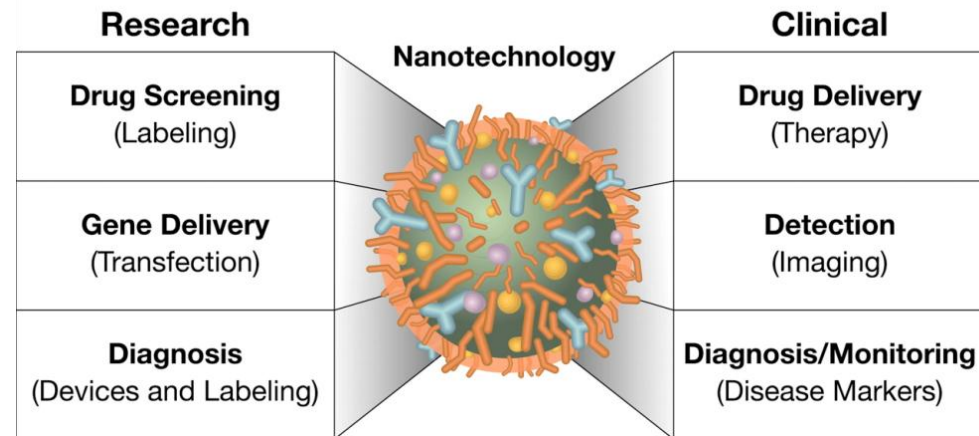
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# What is the problem? *Unrealized potential due to combinatorial complexity*

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



## Medical Applications



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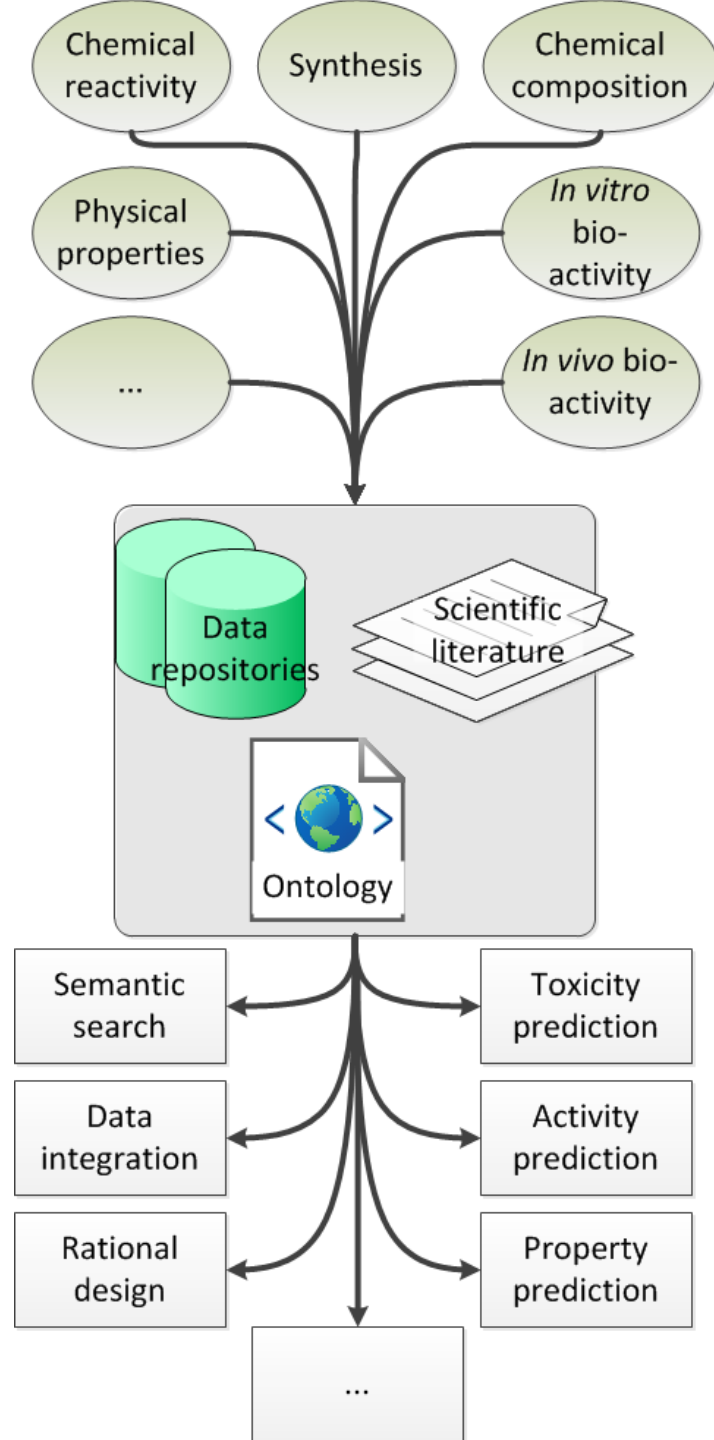
McNeil SE. *J Leukoc Biol*, 2005. **78**(3): p. 585-94.  
doi:10.1189/jlb.0205074

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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



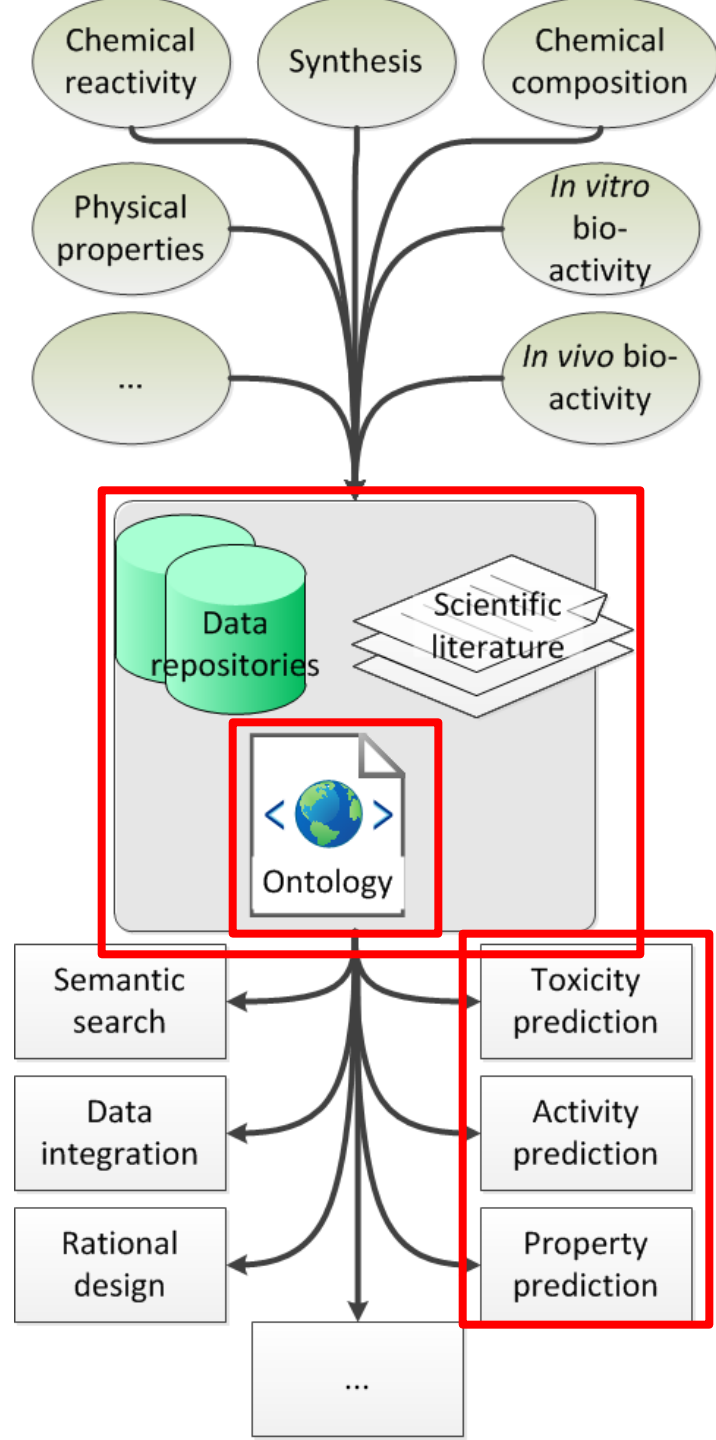
# Our focus

## ► Information exchange and analysis through

- Data exchange standards
- Ontology
- Information resources

## ► Methodology development and applications in nanomaterial prediction:

- Preparation
- Chemical composition
- Physiochemical characterization
- Biological function/behavior





# Outline

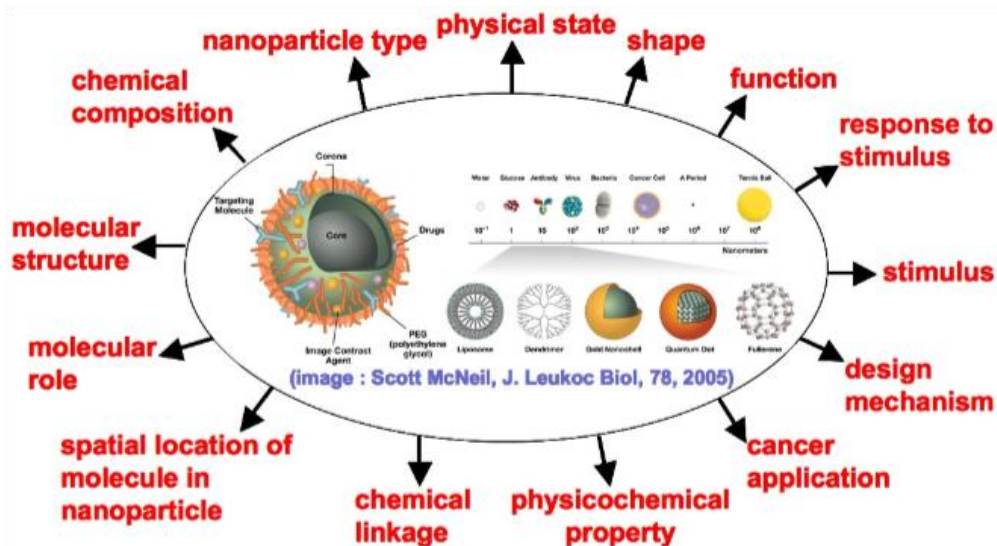
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# NanoParticle Ontology (NPO)



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

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

- ▶ Capture knowledge underlying nanomaterial
  - Preparation
  - Chemical composition
  - Physiochemical characterization
  - Biological function/behavior
- ▶ Basic Formal Ontology structure
- ▶ Initial focus on cancer diagnosis and therapy
- ▶ Tested/validated against
  - Literature and community use cases
  - caNanoLab data
  - Nano WG member datasets
- ▶ Current growth to include a broader range of nanotechnology concepts
- ▶ Supported by the caBIG® Nano WG
- ▶ Multi-disciplinary ***open*** collaborative development

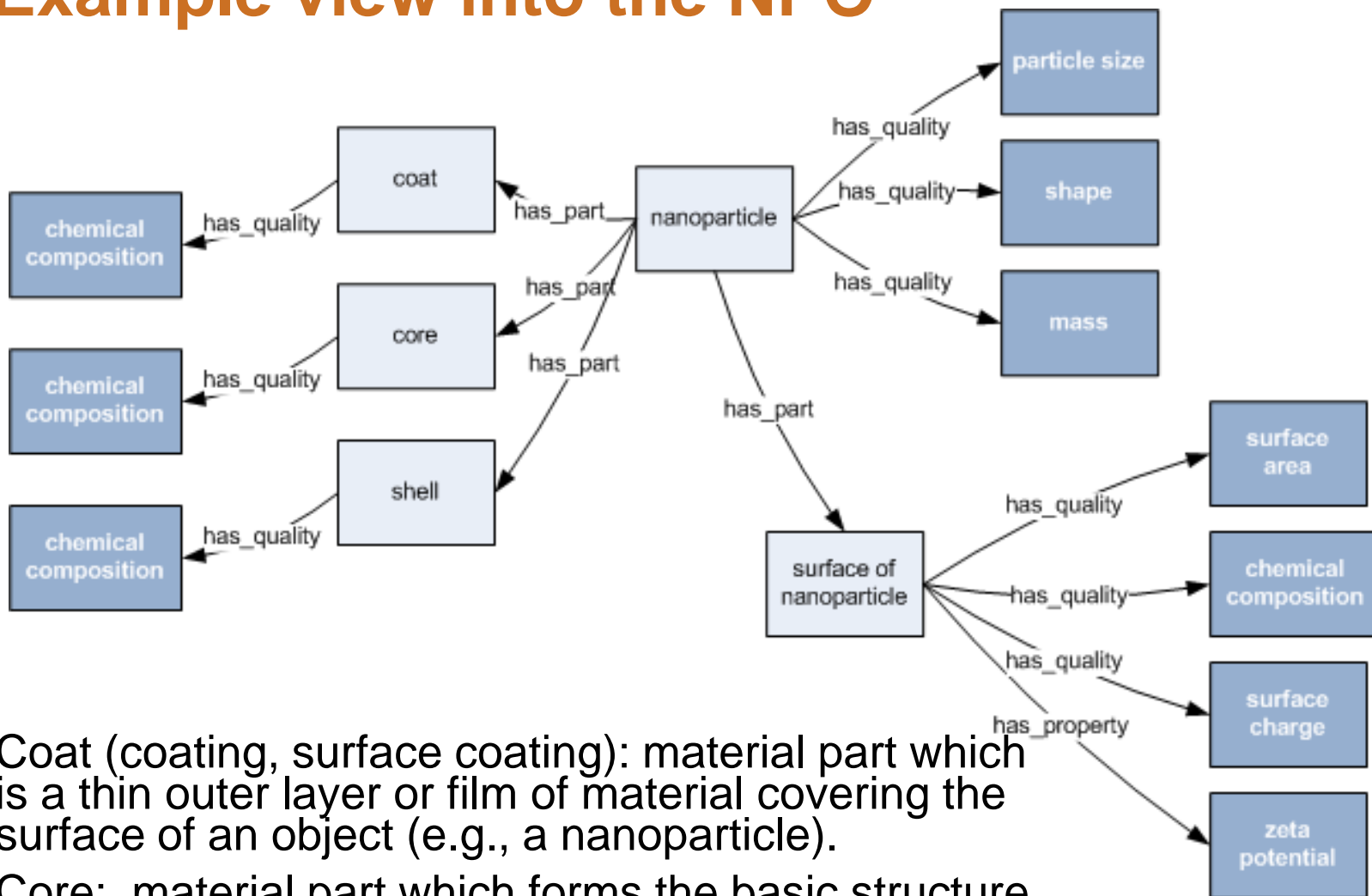
Thomas DG, Pappu RV, Baker NA. NanoParticle Ontology for Cancer Nanotechnology Research. *J Biomed Inform*, in press. doi:[10.1016/j.jbi.2010.03.001](https://doi.org/10.1016/j.jbi.2010.03.001)



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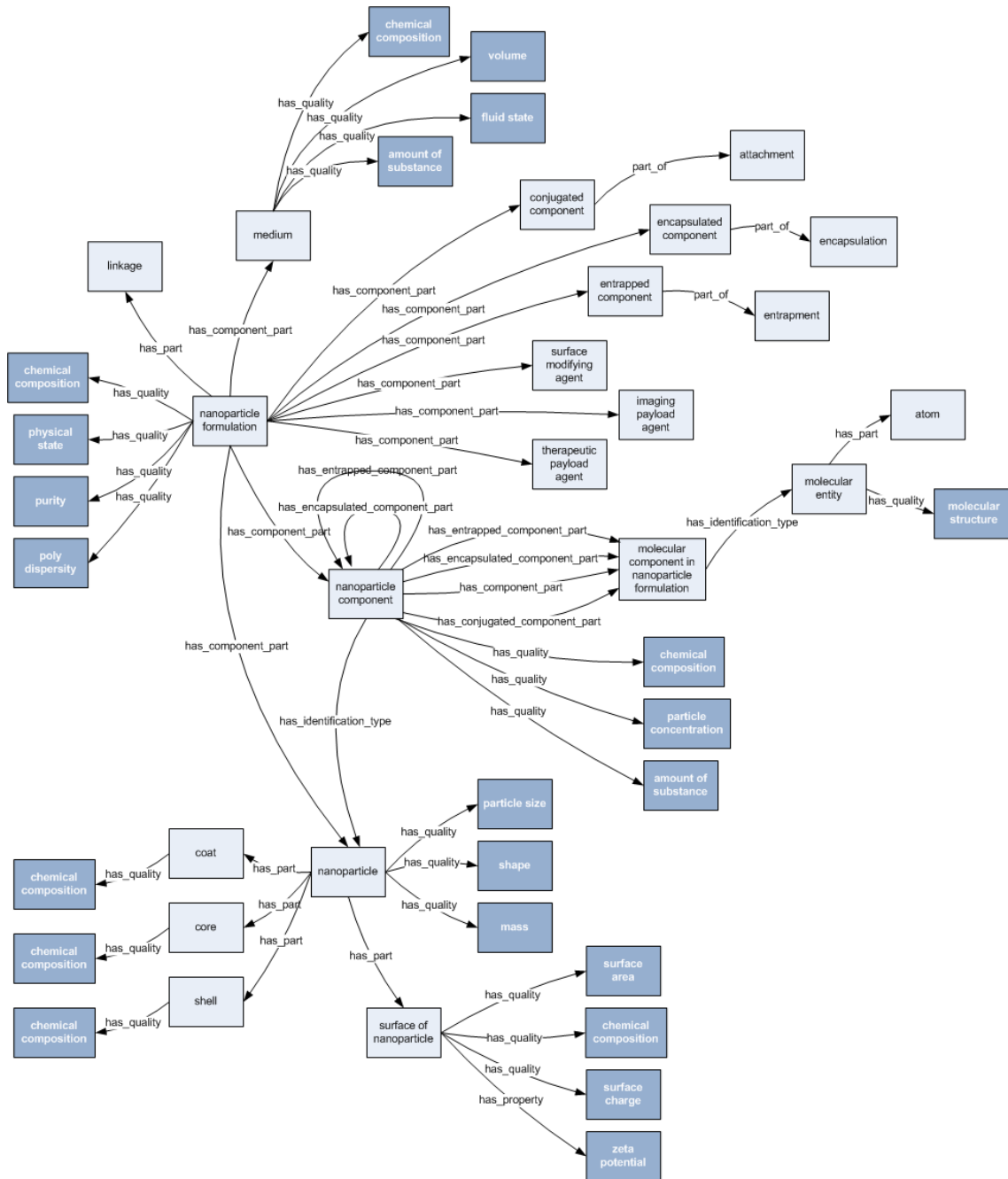
# Example view into the NPO



- ▶ Coat (coating, surface coating): material part which is a thin outer layer or film of material covering the surface of an object (e.g., a nanoparticle).
- ▶ Core: material part which forms the basic structure or central part of an object
- ▶ Shell: material part which is a material layer surrounding the core

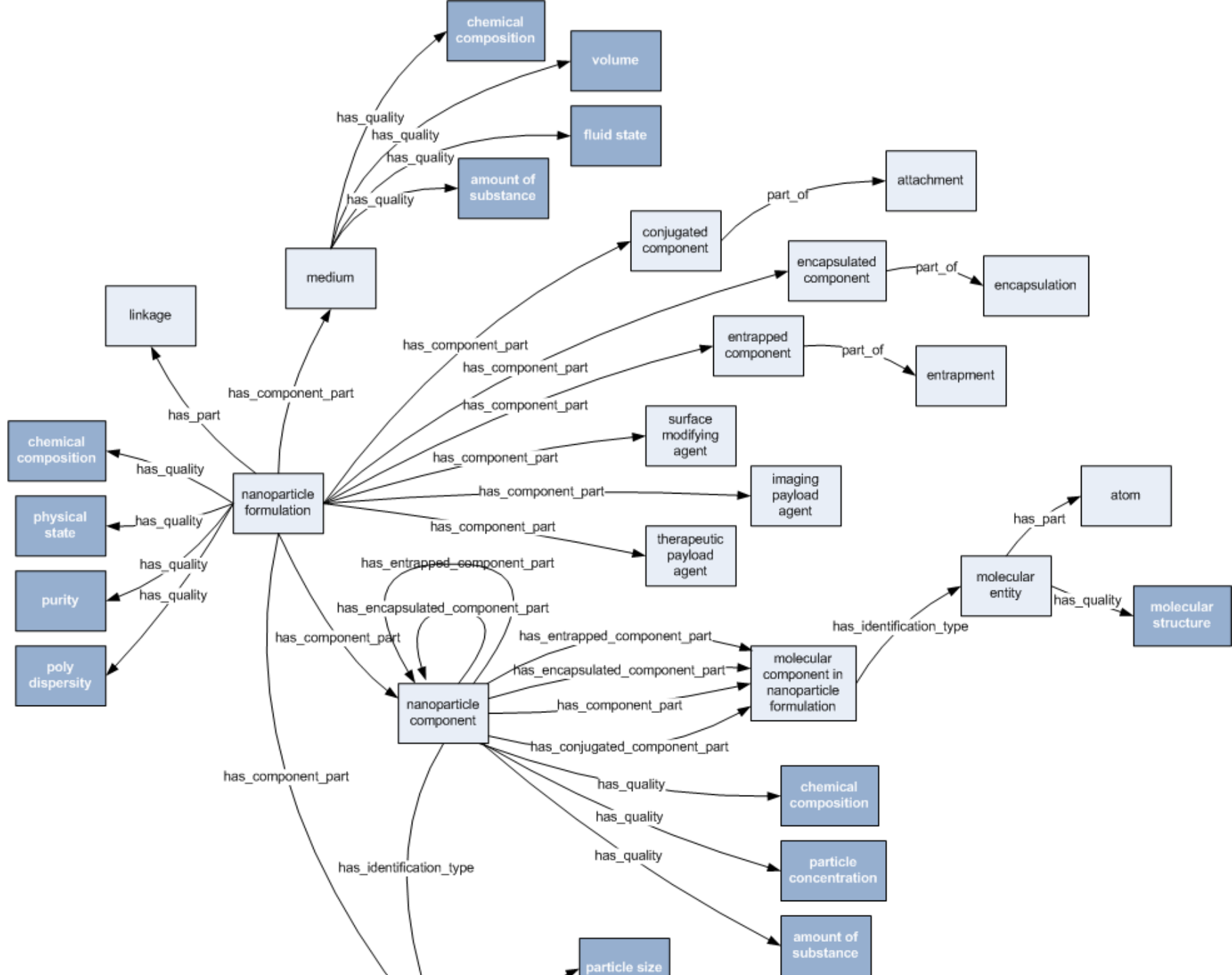


# A more detailed view of nanoparticle composition using the NPO



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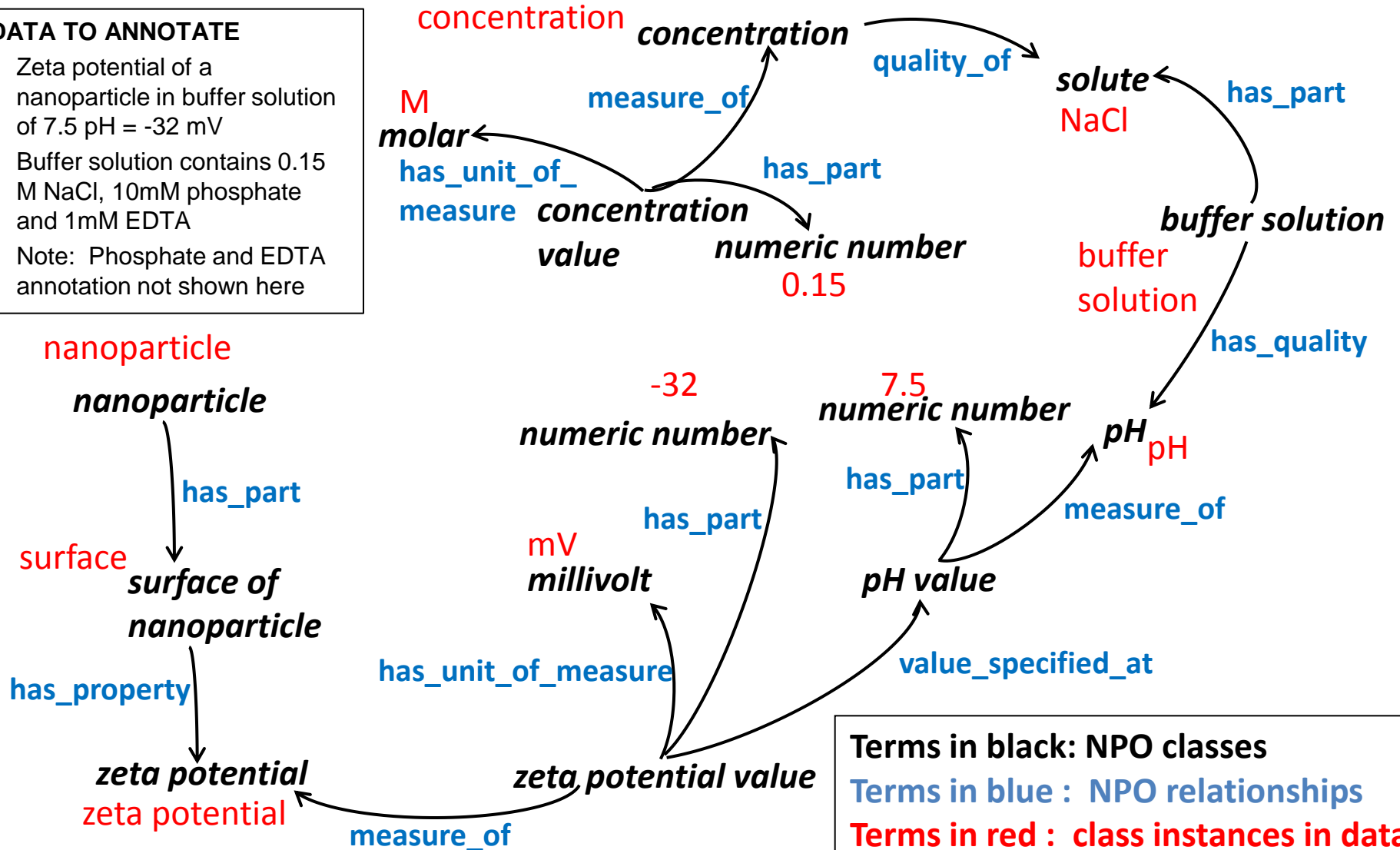
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# Annotation and semantic integration using the NPO

## DATA TO ANNOTATE

- Zeta potential of a nanoparticle in buffer solution of 7.5 pH = -32 mV
- Buffer solution contains 0.15 M NaCl, 10mM phosphate and 1mM EDTA
- Note: Phosphate and EDTA annotation not shown here



Terms in black: NPO classes  
Terms in blue : NPO relationships  
Terms in red : class instances in data

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# ISA-TAB NANO FOR NANOMATERIAL DATA SHARING



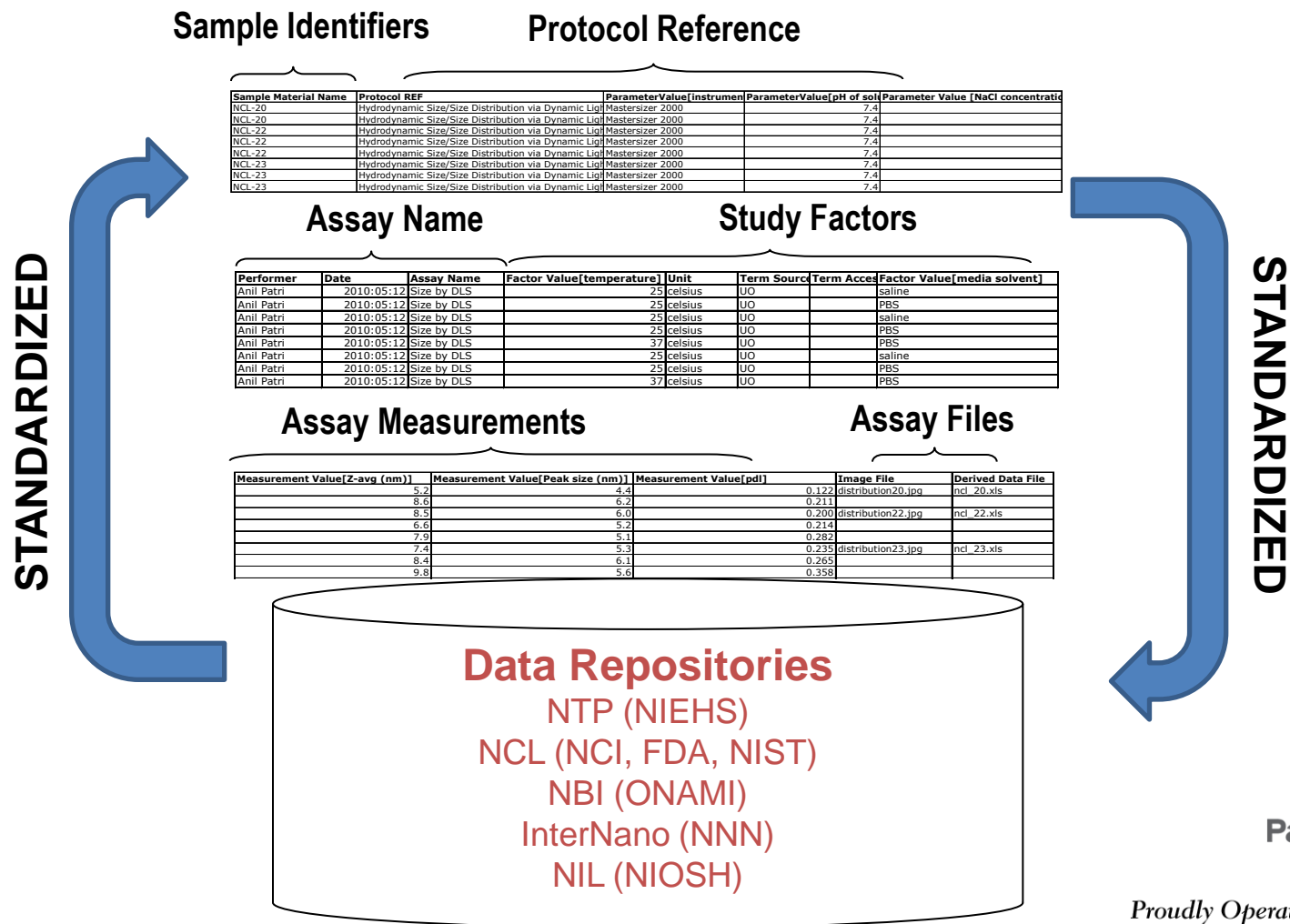
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# Goal of ISA-TAB Nano

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

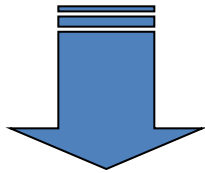


# What is ISA-TAB Nano?

- ▶ 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
- ▶ ISA-TAB Nano supports ontology-based curation
  - Nanomaterials and concepts from the NanoParticle Ontology (NPO) as well as other ontologies

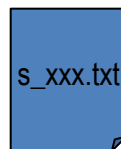
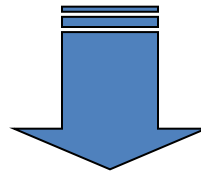
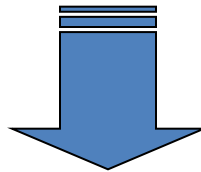
# ISA-TAB Nano structure

**1. Describe the Investigation and Studies**

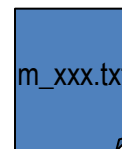


**Investigation File**

**2. Identify Study Samples**

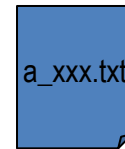
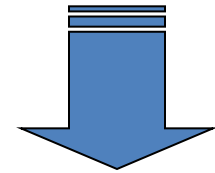


**Study File(s)**



**Material File(s)**

**3. Record Assay Conditions and Measurements**



**Assay File(s)**



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# ISA-TAB Nano 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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# Additional ISA-TAB Nano reading and project team

- ▶ ISA-TAB Nano Project Site: <http://goo.gl/yKFew>
- ▶ ASTM ISA-TAB Nano 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>

## ISA-TAB Nano 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

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## **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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