NPO: Ontology for Cancer Nanotechnology Research

Dennis G. Thomas[1,3], Rohit V. Pappu[1,3] & Nathan A. Baker[2,3]

[1] Department of Biomedical Engineering
[2] Department of Biochemistry and Molecular Biophysics
[3] Center for Computational Biology

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What is NPO (NanoParticle Ontology)?

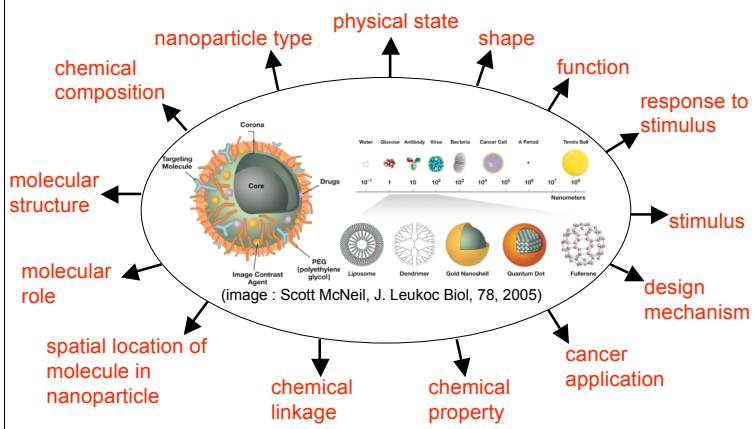
An ontology to represent knowledge underlying the physical, chemical and functional descriptions of nanomaterials which are formulated and tested for cancer diagnostic and therapeutic applications

Why NPO?

To serve as a common vocabulary to:

- annotate disparate and diverse types of nanoparticle data in texts as well as databases to support semantic integration, mining and inferencing of data
- facilitate interdisciplinary discourse in cancer nanotechnology research

Information Used From Peer-Reviewed Journal Articles



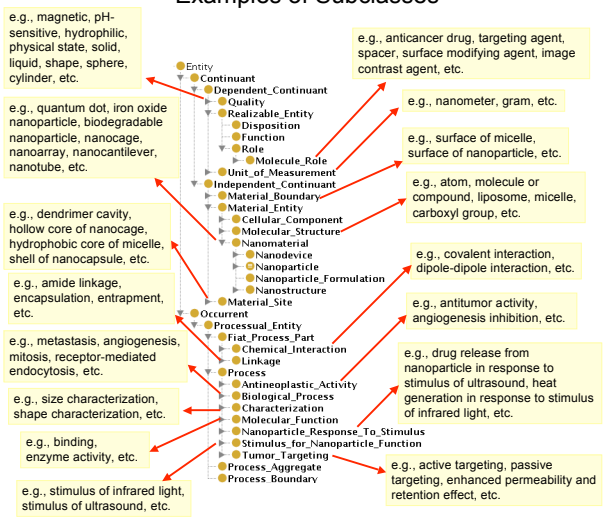
Design Factors for the NPO

- Upper-level classes of the NPO are formed using the Basic Formal Ontology (BFO)
- NPO is expressed in the Ontology Web Language (OWL) using Protégé-OWL editor
- The basic design principles of the NPO are:
  - unbiased entity representation
  - single "is_a" inheritance in asserted OWL hierarchy
  - multiple "is_a" inheritance in inferred OWL hierarchy
  - sibling-disjointedness maintained for BFO classes but not stated at all lower levels in the hierarchy; disjoint axioms applied only between primitive sibling classes at hierarchical levels which have exhausted number of sibling classes
  - provide preferred name, definition, id, synonyms (if any) for each class
  - provide reference ID of classes borrowed from external ontologies / controlled vocabularies (e.g., GO, ChEBI, NCIT)

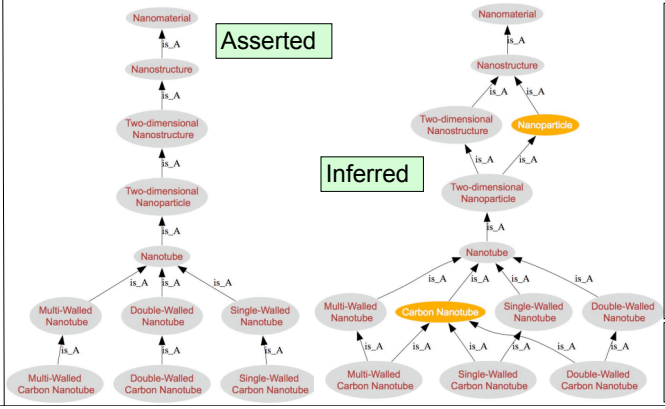
NPO Versions and Release Dates

Version Number	Release Date (mm/dd/yyyy)	No. of OWL classes	No. of OWL object properties (class-level associations)	No. of OWL class annotation properties
2009-06-04	06/04/2009	1270	24	6
2009-04-02	04/02/2009	919	21	6
2008-12-09 beta	12/09/2008	892	21	6
2008-11-20 alpha	11/20/2008	892	21	6
2008-10-20 alpha	10/20/2008	865	22	6
2008-10-16 alpha	10/16/2008	865	22	6

Upper-Level Asserted OWL Class Hierarchy With Examples of Subclasses



is_A Inheritance Example



Class-Level Associations

Name	No. of times used	Usage valid for classes (shown are the top-level classes of these classes)	Examples
has relation to	0	Entity --> Entity	-
part of	69	Continuant --> Continuant Occurrent --> Occurrent	Hollow Core of Nanocage part of Nanocage
has part	237	Continuant --> Continuant Occurrent --> Occurrent	Gold Quantum Dot has part Gold
has component part	21	Nanomaterial --> Molecular Structure Nanomaterial --> Nanomaterial	Chitosan Nanoparticle has component part Chitosan
has conjugated component part	0	Nanomaterial --> Molecular Structure Nanomaterial --> Nanomaterial	-
has encapsulated component part	0	Nanomaterial --> Molecular Structure Nanomaterial --> Nanomaterial	-
has entrapped component part	1	Nanomaterial --> Molecular Structure Nanomaterial --> Nanomaterial	Gold Quantum Dot-Entrapped Polyamidoamine Dendrimer Nanoparticle has entrapped component part (Gold Quantum Dot and participates in Entrapment)
is integral part of	112	Atom --> Element	Carbon Atom is integral part of Carbon
has quality	67	Continuant --> Quality Occurrent --> Quality	Biodegradable Nanoparticle has quality Biodegradable
has role	64	Molecular Structure --> Molecule Role	Doxorubicin has role Topoisomerase-II Inhibitor
stimulus causes response	3	Stimulus For Nanoparticle Function --> Nanoparticle Response To Stimulus	Stimulus Of Infrared Light stimulus causes response Nanoparticle Response To Infrared Light
has function realized as process	8	Molecule Role --> Occurrent Material Entity --> Occurrent	Angiogenesis Inhibitor has function realized as process Angiogenesis Inhibition
inhibits	17	Molecule Role --> Occurrent Material Entity --> Occurrent	Topoisomerase-II Inhibitor inhibits DNA Topoisomerase II Activity
regulates	1	Molecule Role --> Occurrent Material Entity --> Occurrent	DNA-RNA Transcription Regulator regulates DNA-Dependent Transcription
has participant	50	Occurrent --> Material Entity Occurrent --> Molecule Role	Amide Linkage Between Primary Amine and Carboxylic Acid has participant Primary Amine Group; has participant Carboxyl Group
has output participant	22	Occurrent --> Material Entity Occurrent --> Molecule Role	Amide Linkage Between Primary Amine and Carboxylic Acid has output participant Carboxamide Group
participates in	4	Material Entity --> Occurrent Molecule Role --> Occurrent	Gold Quantum Dot-Entrapped Polyamidoamine Dendrimer Nanoparticle has component part (Polyamidoamine Dendrimer and participates in Entrapment)
describes property	5	Characterization --> Quality	Size Characterization describes property Size
has unit of measure	39	Quality --> Unit Of Measurement	Length has unit of measure Length Unit
unit of	31	Unit Of Measurement --> Quality	Length Unit unit of Length
has bond with	2	between Atom classes which are part of a Polyatomic Entity class	Organonitrogen Compound has part (Carbon Atom and has bond with Nitrogen Atom)
has single bond with	2	between Atom classes which are part of a Polyatomic Entity class	Chlorambucil has part (Carbon Atom and has single bond with Chlorine Atom)
has double bond with	0	between Atom classes which are part of a Polyatomic Entity class	-
has triple bond with	0	between Atom classes which are part of a Polyatomic Entity class	-

Conclusions and Future Directions

- Evaluate classes (name, synonyms, definitions, is_A classification) and enrich the NPO
- Expand scope based on user needs and feedback (caNanoLab)
- Achieve caBIG compatibility
- Establish governance structure with community effort for maintenance, review and development of the ontology
- Public releases of NPO are available through BioPortal (http://bioportal.bioontology.org/virtual/1083)
- NPO uploaded at BiomedGT Wiki for collaborative ontology development (http://tinyurl.com/npo-biomedgt)
- NPO documentation available at http://npo.wustl.edu

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