

National Cancer Institute (NCI) National Cancer Informatics Program (NCIP) Nanotechnology Working Group

<https://wiki.nci.nih.gov/display/ICR/Nanotechnology+Working+Group>

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Long-term goals

This Working Group is motivated by two high-priority nanomedicine informatics applications:

- The rational design of nanomaterials customized for use in nanomedicine, including therapeutic, diagnostic, and preventative applications.
- The development of robust structure-activity relationships to predict the biological effects associated with nanomaterials and to utilize this insight for medical applications and/or to reduce hazards to health, safety and the environment.

These applications will be enabled by broad computational capability applied to nanotechnology research. The development of such capability has led to the following long-term objectives for the Nano WG:

- To enable nanomedicine data search, sharing, and analysis through ontology development.
 - One project directly related to this goal is the NanoParticle Ontology: <http://nano-ontology.org>
- To establish common framework for describing and accessing the physiochemical and biological data of nanotechnology using common data elements and data sharing formats.
 - One project directly derived from this goal is the ISA-TAB-Nano standard for data submission: <http://is.gd/foSKV>

- To develop a framework for uniform and comprehensive data curation and annotation ensuring that data reliability and reproducibility is evaluated by users most familiar with both the data and the methods used to produce it.
- To encourage the development of effective data mining standards and tools that are particularly suited for nanomaterial safety assessment safe-by-design approaches, establishing nanotoxicology structure-activity relationships and nanomaterials characterization databases used for accompanying these objectives.
- To encourage adoption and use of a shared informatics infrastructure by the nanotechnology and broader communities.

Short-term aims

To realize the long-term objectives outlined above, the NCIP Nano WG has established several short-term goals with 6-12 month timeframes.

Aim 1. Descriptive analytics for nanomaterial-biological interactions

We will work to identify datasets and develop statistical analytic models that help to identify the key features that describe the biological activity of selected nanomaterials. The main challenge is a lack of large high quality datasets to support predictive modeling. Datasets that are incomplete, lack validation, or are low quality are considered to be in the 'incubator phase' to ensure that we do not delude the quality of data for informatics. However, the data currently available in such incubators can be used to discover interesting trends (generate hypotheses) to guide development of new approaches for both the characterization of nanomaterials and the modeling. We recognize that diverse nanoparticles with different cores and surface modifiers tested for specific biological activity can be characterized by experimental physical, geometrical, and electronic properties to enable modeling; alternatively, nanoparticles with the same core but different surface modifiers can be characterized by computed chemical descriptors of these modifiers. The goals of this activity will be to (1) collect and standardize experimental properties of nanoparticles (which will also fuel ontology development under Aim 2, vide infra), (2) develop novel approaches to computing descriptors of chemical, physical, geometrical, and electronic properties of nanoparticles, and (3) develop predictive models of nanoparticles' biological activity that can be interpreted to elucidate activity-defining features and obtain mechanistic insight into nanomaterial biological activity. Specific tasks will include:

- a) Survey of existing datasets for potential analysis and collaboration
- b) Analysis of specific datasets made available to the working group:
 - i. Stacey Harper's embryonic zebrafish nanomaterial toxicity dataset.
 - ii. Dennis Hourcade's and Christine Pham's nanomaterial complement activation dataset.
 - iii. Amiji Mansoor's halyuronic acid nanoparticle dataset.

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Comment [1]: Requires Wash group's agreements and terms/conditions

Nathan Baker 10/3/12 12:12 PM

Comment [2]: Requires Mansoor group's agreements and terms/conditions

- iv. Bing Yan's set of decorated nanotubes previously studied by Denis Fourches and Alex Tropsha.

Where sufficient data is available, we will identify priorities and next steps for predictive modeling of nanomaterial biological activity.

Aim 2. Continued nanotechnology ontology development

Data generated from nanotechnology research are so diverse and large in volume that it is difficult to share and efficiently use them without informatics tools. In particular, ontologies that provide a unifying knowledge framework for annotating the data are required to facilitate the semantic integration, knowledge-based searching, unambiguous interpretation, mining and inferencing of the data using informatics methods. The Nano WG supports the continuing development and application of the NanoParticle Ontology (NPO), which is developed within the framework of the Basic Formal Ontology (BFO), and implemented in the Ontology Web Language (OWL) using well-defined ontology design principles. Nano WG will work closely with data repositories and data curation efforts to capture requirements and incorporate new terminology in NPO. See <http://nano-ontology.org> for more information. Work on this aim will consist of the following tasks:

- a) Identify NPO requirements through regular interactions or collaborations with the Nanomaterial Registry, the US-EU Community of Research on Databases and Ontology, CEIN, CEINT, the National Nanomanufacturing Network and other interested parties.
- b) Grow the NPO through identification and definition of additional concepts in Task and incorporate those concepts into the NPO.

Aim 3. Continued data sharing standard development

ISA-TAB-Nano was developed to facilitate the import and export of data on nanomaterials and their characterizations among nanotechnology resources. Nano WG will continue to update the specification based on the feedback from the community. Nano WG will also continue to work with the [ISA-team](#) to extend the ISA-TAB validator to support ISA-TAB-Nano extensions, and to explore the use of ISA OntoMaton that allows users to search for ontology terms while annotating their experiments. The ISA-TAB-Nano project is under development as an ASTM standard (WK28974 at <http://is.gd/foSKV>). See the [ISA-TAB-Nano Specification](#) for more information. Work on this Aim will be focused on the following tasks:

- a) Nano WG will continue to reach out to the community to increase awareness of the resources developed by the Nano WG, and to encourage community participation in the WG activities. In particular, the following activities will be leveraged to increase participation: invitations to program officers with nanotechnology portfolios, announcements and invitations via the nano.gov portal, society presentations (e.g. Society of Toxicology Nanotoxicology Specialty Section, Society for Environmental Toxicology and Chemistry); and present posters on WG activities at conferences and meetings.

Nathan Baker 10/10/12 7:07 AM

Comment [3]: Requires Bing Yan's agreement for release to the WG

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Comment [4]: Pending Michelle's agreement

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- b) Additional templates and examples will be developed based on community needs and feedback.
- c) The ISA-TAB-Nano standard will continue to be developed/modified based on user feedback and interaction with the ISA-Tools community.
- d) Time permitting, we will explore the extension of ISA-TAB formats to the sharing of nanotechnology models in addition to the current data sharing activities.

In the course of these activities, we also plan to survey and identify issues in nanotechnology data curation and search that should be standardized across data resources.