Nanotechnology Working Group

Participation and Communication

The NCI Nanotechnology Working Group is a working closely with the Nanotechnology community, and working group calls are open to anyone interested in participating in and contributing to the working group discussions and activities.

Group communications are managed through the NCI Community Hub and the Nano-Standards listserv.

Meeting Information

Nano WG meetings will take place on every Thursday at 11 am ET

- **Web conference**: Webex link
  Meeting password: Technology1!

Audio:

Join by phone
1-855-244-8681 Call-in toll-free number (US/Canada)
1-650-479-3207 Call-in toll number (US/Canada)
Access code: 739 206 220

Nano WG Meeting Schedule

Nano WG meeting calendar has moved to the NCIP Hub https://nciphub.org/groups/nanowg/calendar/2014/06

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Mission Statement

The National Cancer Institute (NCI) National Cancer Informatics Program (NCIP) Nanotechnology Working Group was established in 2008 for researchers with a specific interest in informatics and computational approaches to nanotechnology, with a particular emphasis on nanomedicine. The goal of this working group is to demonstrate the scientific potential of federating nanotechnology databases through pilot projects aimed at integrated semantic search and retrieval of nanomedicine and nanotoxicology datasets that are applicable across nanoscience. The NCIP Nanotechnology Working Group (NCIP Nano WG) comprises over 20 active participants from academia, government and industry with diverse interests.

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 preventive applications.
- The development of robust and validated structure-activity relationships to predict the biological effects associated with nanomaterials and to utilize this insight for medical applications and/or to reduce hazards, exposures, and resulting risks 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 a common framework for describing and accessing the physiochemical and biological properties 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 dilute 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 approaches to identifying 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:

1. Survey of existing datasets for potential analysis and collaboration; define important attributes for datasets of interest.
    a. Datasets generated by Investigators from the NCI Alliance for Nanotechnology
2. Analysis of specific datasets made available to the working group:
    a. Stacey Harper's embryonic zebrafish nanomaterial toxicity dataset.
    b. Other datasets to be identified by the group in Task (a).

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

Proposed Data Sharing "Ground Rules" for Data Analyzed by the Nano WG: NanoWG_DataSharing.pptx

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:

1. Identify NPO requirements through regular interactions or collaborations with the Nanomaterial Registry, the US-EU Community of Research on Databases and Ontology, UC CEIN, CEINT, the National Nanomanufacturing Network, and other interested parties.
2. Grow the NPO through identification and definition of additional concepts in Task A 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:

1. 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.
2. Additional templates and examples will be developed based on community needs and feedback to improve overall usability and to facilitate adoption of the ISA-Tools.
3. The ISA-TAB-Nano standard will continue to be developed/modified based on user feedback and interaction with the ISA-Tools community.
4. 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.

Completed

See Nanocharacterization Library

Standardizing nanomaterial characterization protocols. Several Working Group members have noted that standard characterizations discussed above are only useful if the protocols for these characterizations are themselves standardized and reproducible. Furthermore, evidence from inter-laboratory studies by ASTM and IANH suggests that there is significant variability in results from existing "standard" protocols, suggesting that current mechanisms for protocol communication are ineffective. This nanotechnology problem is currently under investigation by ASTM and ISO groups. The Working Group assists in this effort by:

- Collecting standard methodologies related to the characterization activities described above.
- Providing a forum with a diverse group of participants for discussing the best mechanisms for sharing nanotechnology characterization protocols.
- Augmenting data with computational data.

Ongoing

Defining standards for nanomedicine data sharing and exchange. Currently, access to relevant data is a major barrier to the realization of the nanomedical goals of rational nanomaterial design and toxicity prediction. While a few detailed datasets exist for nanomaterial toxicity (ONAMI), and nanomaterial-cellular interactions (Shaw and others) most of the necessary data is dispersed across a wide array of nanotechnology data resources. Therefore, it is essential to implement an infrastructure to ensure that these data can be shared among researchers and data resources. To develop this (federated) data sharing infrastructure, the Working Group has undertaken development of the ISA-TAB-Nano spreadsheet form, based on the ISA-TAB framework, to facilitate submission of data by experimental researchers. The ISA-TAB-Nano effort is translating the great success of MAGE-TAB microarray and similar formats for enabling data sharing in other communities. Ongoing development is based on community requirements and feedback: See ISA-TAB-Nano Specification

Providing vocabulary and semantic support to the nanomedicine community. 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 NCIP Nano WG supports the continuing development and application the of 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. The NPO was developed to represent knowledge underlying the preparation, chemical composition and characterization of nanomaterials involved in research.

Ongoing development based on community requirements and feedback

More information can be found at http://nano-ontology.org