

Nanoinformatics at NIH

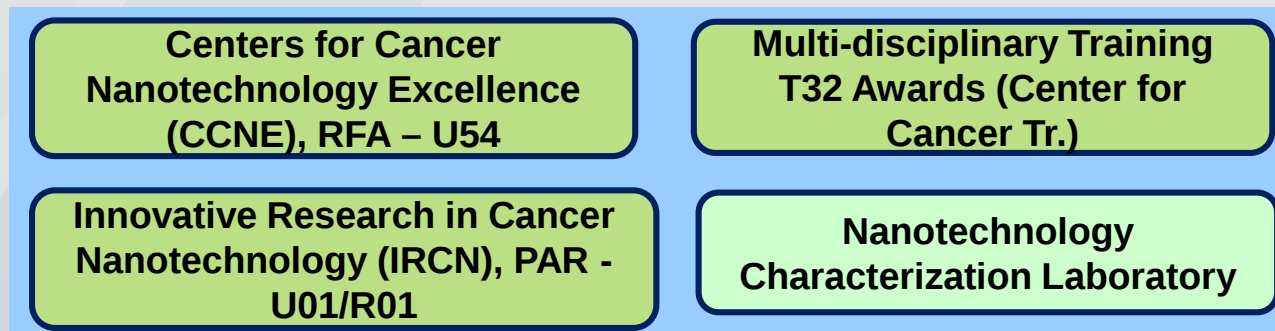
National Nanotechnology Initiative: Quadrennial Review Meeting #1

Stephanie Morris, PhD
Office of Strategic Coordination
National Institutes of Health, Office of the Director

Who I am, Why I am Here

- Current—Extramural Research Program Officer in the National Institutes Office of the Director, Office of Strategic Coordination (Common Fund Office) (<1 year)
- Recent—Extramural Research Program Director at the National Cancer Institute/National Institutes of Health (6 years)
 - The Nanodelivery Systems and Devices Branch within the NCI's Division of Cancer Treatment and Diagnosis
- Part of team overseeing NCI's Alliance for Nanotechnology in Cancer (Alliance) program
 - Focused on the development and application of nanotechnology to cancer—imaging, early detection, and treatment

Phase 3 Alliance Program, 2015-2020

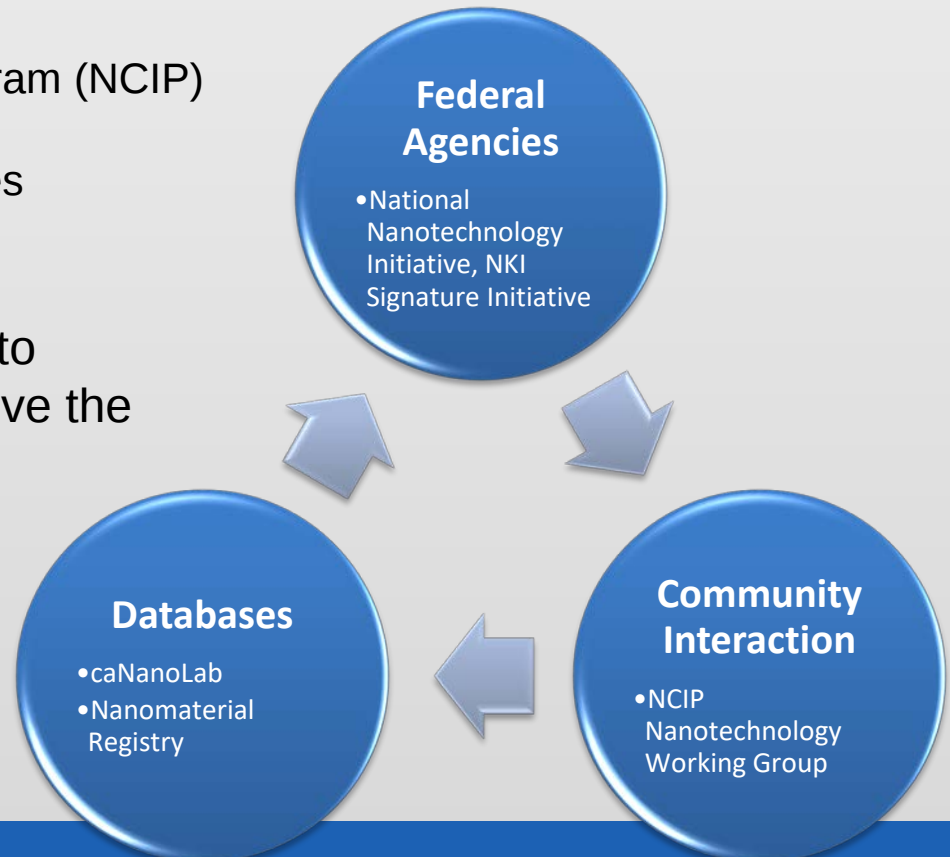


- NIH has one of the largest budgets dedicated to support of nanotechnology-based biomedical research—NCI, NIAID, NIDCR, NIEHS, and NIBIB

Who I am, Why I am Here

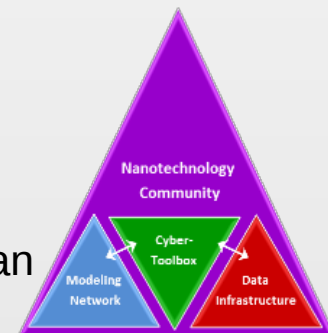
- Promote biomedical nanotechnology resources by interacting with other research programs, federal agencies, and the wider community
- NIH is a participating agency of the National Nanotechnology Initiative
 - NSI on Nanotechnology for Sensors and Sensors for Nanotechnology (Dorothy Farrell, Christopher Hartshorn, NCI)
 - NSI on Nanotechnology Knowledge Infrastructure (James Luo, NIBIB; George Hinkal, Stephanie Morris, Christina Liu, NCI)
 - National Cancer Informatics Program (NCIP) Nano Working Group
 - Support of nanomaterial databases

NCI and the broader NIH realize the importance of data sharing and re-use to enable knowledge discovery and improve the rational design of nanomaterials



Nanotechnology Knowledge Infrastructure (NKI)

Global Challenge: With new innovations in nanotechnology and engineered nanomaterials, and the funding and application of nanotechnology to varied disciplines (biomedicine, EHS, energy, etc.), we are seeing an increase in the amount and diversity of the underlying data. As with other scientific disciplines, an informatics infrastructure is needed to integrate this new knowledge to improve data sharing, data quality, reproducibility, and data analysis and modeling to further enable rationale nanomaterial design.



NKI Purpose: To provide a community-based, solutions-oriented knowledge infrastructure to accelerate nanotechnology discovery and innovation.

- Launched in 2012; 4th NNI signature initiative
- Eleven participating agencies:



<http://www.nano.gov/NKIPortal>

NKI Thrust Areas

- A **diverse collaborative community** of scientists, engineers, and technical staff to support research, development, and applications of nanotechnology to meet national challenges
- An **agile modeling network** for multidisciplinary intellectual collaboration that effectively couples experimental basic research, modeling, and applications development
- A **sustainable cyber-toolbox** to enable effective application of models and knowledge to nanomaterials design
- A **robust** digital nanotechnology **data and information infrastructure** to support effective data sharing, collaboration, and innovation across disciplines and applications

Example Key Challenges to Address

- Data sharing
 - Accessible and sustainable databases; Appropriate metadata; Format
- Ontologies and nomenclature
- Data reproducibility, reliability, and validation
 - Role of journals; Standardizing protocols; Uncertainty quantification
- Database federation and interoperability
 - Uniting diverse datasets with similar interests
- Comparing and validating models
- Training

Most importantly, bringing together the various ongoing efforts and programs:

CODATA-VAMAS, MGI, InterNano, CEINT Knowledge Commons, NanoHUB, NKI, NCIP Nanotechnology Working Group, caNanoLab, US-EU Communities of Research, EU Nanosafety Cluster, etc.

Thrust 1—Build a Diverse Collaborative Community

A **diverse collaborative community** of scientists, engineers, and technical staff to support research, development, and applications of nanotechnology to meet national challenges. Working towards that by:

- Participating in and organizing workshops on nanoinformatics, especially at meetings focused on nanotechnology
- Sharing NKI activities with the broader nanotechnology community at conferences/meetings with grantees, hosting sessions and giving presentations that highlight efforts of NKI
- and, importantly, working with other initiatives and working groups
 - Materials Genome Initiative
 - U.S.-EU Communities of Research
 - NCIP Nanotechnology Working Group (NCIP Nano WG)

- 2016 NanoEHS Workshop—"Enabling a sustainable harmonised knowledge infrastructure supporting nano environmental and health safety assessment"
 - Organized to support ongoing US-EU dialogue in the area of NanoEHS with the goal of encouraging joint projects
 - Chaired by Barry Hardy (OpenTox Association) and Lisa Friedersdorf
- 2017 Cancer Nanotechnology Gordon Research Conference Session—"Nanoinformatics, Rational Design, Modeling and Simulation"
 - Introduced nanoinformatics to participants as a means to enhance reproducibility and rigor, nanomedicine design, and data management
 - Chaired by Alex Tropsha (UNC-Chapel Hill)
- 2018 NNI Public Webinar Series—"NanoEHS and Nanomedicine: Similarities and Synergism"
 - Chaired by Christina Liu (NIH) and Mark Hoover (NIOSH)
 - Panelists from both areas gave a comparative overview of their respective disciplines and discussed how each field's tools and developments can inform each other and tackle common challenges
- Upcoming 2019 Symposium at the American Chemical Society National Meeting & Exposition—"Nanoinformatics: Information and Data Sciences Applied to Nanomaterials Synthesis, Properties, and Biological Effects"

- 2016 NanoEHS Workshop—“Enabling a sustainable harmonised knowledge infrastructure supporting nano environmental and health safety assessment”
 - Organized to support ongoing US-EU dialogue in the area of NanoEHS with the goal of encouraging joint projects
 - Chaired by Barry Hardy (OpenTox Association) and Lisa Friedersdorf
- 2017 Cancer Nanotechnology Gordon Research Conference Session—“Nanoinformatics, Rational Design, Modeling and Simulation”
 - Introduced nanoinformatics to participants as a means to enhance reproducibility and rigor, nanomedicine design, and data management
 - Chaired by Alex Tropsha (UNC-Chapel Hill)
- 2018 NNI Public Webinar Series—“NanoEHS and Nanomedicine: Similarities and Synergism”
 - Chaired by Christina Liu (NIH) and Mark Hoover (NIOSH)
 - Panelists from both areas gave a comparative overview of their respective disciplines and discussed how each field’s tools and developments can inform each other and tackle common challenges
- Upcoming 2019 Symposium at the American Chemical Society National Meeting & Exposition—“Nanoinformatics: Information and Data Sciences Applied to Nanomaterials Synthesis, Properties, and Biological Effects”

2016 NanoEHS Workshop—"Enabling a sustainable harmonised knowledge infrastructure supporting nano environmental and health safety assessment"

- As part of this meeting, one of the first in-person discussions about the EU US Roadmap Nanoinformatics 2030 (Published November 2018, DOI: 10.5281/zenodo.1486012)
 - Editors: Andrea Haase (German Federal Institute for Risk Assessment) and Fred Klaessig (Pennsylvania Bio Nano Systems)
 - Focus on broad overview of nanoinformatics as well as regulatory acceptance of computational models for risk assessment
 - Many involved in putting this together: US-EU Communities of Research, EU Nanosafety Cluster, and the NCIP Nanotechnology Working Group

The screenshot shows the Zenodo page for the publication "EU US Roadmap Nanoinformatics 2030". The page is dated November 15, 2018, and is marked as "Open Access". The title is prominently displayed at the top. Below the title, the authors are listed as Haase and Klaessig. A summary paragraph states that the roadmap was jointly developed by scientists from the European Union, the United States, and a few other countries, with the main purpose being educational. It also includes a disclaimer that the opinions expressed are solely those of the authors and do not represent the official policy of their respective governments. The page features a sidebar on the right with statistics: 519 views, 456 downloads, 7 tweets, and 10 readers on Mendeley. It also shows the publication date, DOI (10.5281/zenodo.1486012), and keywords (Nanoinformatics, Roadmap, EU Nanosafety Cluster, EU, USA). A preview of the document is shown at the bottom, displaying the title "EU US Roadmap Nanoinformatics 2030" on a white background.

November 15, 2018

Other Open Access

EU US Roadmap Nanoinformatics 2030

Haase; Klaessig

This roadmap has been jointly developed in trustful cooperation among scientists of the European Union, the United States of America and a few other countries. Scientists with different scientific backgrounds, working in the field of nanotechnology, have cooperated with the main objective to provide as broad an overview as possible about the young and rapidly evolving field of "nanoinformatics". Thus, the main purpose of this roadmap is educational. By no means was the intention to provide all possible details. Instead, interested readers will find plenty of additional references mentioned in each of the chapters that will provide more detailed insights.

The opinions expressed in this document are solely those of the authors. They do not necessarily represent the opinions of their respective organisations or reflect the views, and official policy of the respective Government such as the Department of Defence, the Department of the Army, the U.S. Army Medical Department or the U.S. Federal Government. Mention and use of product or trademark name(s) does not constitute endorsement but is intended only to assist the reader.

The statements and opinions contained in the individual chapters are also not legally binding with respect to different regulatory frameworks. In particular it should be noted that some of the terms might be defined and used differently in the US versus the EU, also within different scientific disciplines and within different regulatory frameworks. Therefore, within the definitions sections we attempted to provide an overview, to explain the most important terms, and to highlight some that may have different meanings.

519 views 456 downloads

See more details...

7 Tweets by 9 10 readers on Mendeley

See more details

Indexed in

OpenAIRE

Publication date: November 15, 2018

DOI: DOI 10.5281/zenodo.1486012

Keyword(s): Nanoinformatics Roadmap EU Nanosafety Cluster EU USA

Imprint: EU Nanosafety Cluster.

Communities: EU NanoSafety Cluster

License (for files): Creative Commons Attribution 4.0 International

Preview

Page: 1 of 126 Automatic Zoom:

EU US Roadmap Nanoinformatics 2030

2017 Cancer Nanotechnology Gordon Research Conference Session— "Nanoinformatics, Rational Design, Modeling and Simulation"

- Introduced nanoinformatics to participants as a means to enhance reproducibility and rigor, nanomedicine design, and data management—the first time a session like this has been held at the Cancer Nanotechnology Meeting
- Organized by Alex Tropsha, meeting chairs, and NCI

7:30 pm - 9:30 pm	Nanoinformatics, Rational Design, Modeling and Simulation Discussion Leader: Alexander Tropsha (University of North Carolina at Chapel Hill, USA)
7:30 pm - 8:10 pm	Fred Prior (University of Arkansas for Medical Sciences, USA) Dan Heller (MSKCC) "Informatics to Enhance Rigor and Transparency in Nanomedicine Research"
8:10 pm - 8:30 pm	Discussion
8:30 pm - 9:10 pm	Stephanie Morris (National Cancer Institute, NIH, USA) and Chiara Pastore (Nature Nanotechnology, United Kingdom) "Informatics and Data Management in Nanomedicine"

Outcomes:

- Increased participation of nanomedicine researchers in the NCIP Nanotechnology Working Group—Dan Heller, Luisa Russell, and several others.
- Later that summer, Dan Heller proposes to organize a a nanoinformatics symposium at the National American Chemical Society meeting (Fall 2019 in San Diego)
- Introduction to an electronic Nanobook

Cancer Nanotechnology
Gordon Research Conference

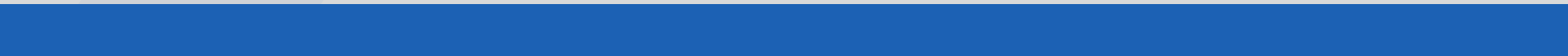
Multimodal Nano-Therapies Against Cancer
June 18 - 23, 2017

Chairs
Alexander V. Kabanov

Vice Chair
Ronit Satchi-Fainaro

Mount Snow
89 Grand Summit Way
West Dover, VT, US

Venue and Travel Information



2019 Symposium at the American Chemical Society Meeting—"Nanoinformatics: Information and Data Sciences Applied to Nanomaterials Synthesis, Properties, and Biological Effects"

- August 25 - 29, 2019, San Diego, CA. Division of Colloid and Surface Chemistry [COLL]
- Organized by Dan Heller (MSKCC/Weill Cornell Med), James Dahlman (Georgia Tech/Emory), Shan Jiang (Iowa State), and Avi Schroeder (Technion Israel Institute of Technology)
- This session will focus on the use of data science and information science in the development and understanding of nanomaterials and nanomedicines. Topics include, but are not limited to:
 - Machine learning applied to nanotechnology
 - Information management related to nanomaterials
 - Data mining approaches
 - Data standardization in nanotoxicology
 - Data homogeneity in nanomaterials characterization
 - Chemical information applied to nanoscience
- Confirmed Invited Speakers
 - Chad Mirkin – Northwestern University
 - Luisa Russell – National Cancer Institute
 - Bryce Meredig – Citrine Informatics
 - Aravind Asokan - Duke University
 - Korin Wheeler - Santa Clara University
 - Giuseppe Battaglia - University College London
 - Eric Shapiro - Michigan State University
 - Yosi Shamay – Technion - Israel Institute of Technology
 - Rein Ulijn – City University of New York

NCIP Nanotechnology Working Group (NCIP Nano WG)

- Initiated in 2008 as an open, informal working group, with the objectives of:
- Developing data exchange standards and ontologies
- Building a community of practice around nano-data reuse and integration to support:
 - Predictive models for nanomaterial activity
 - Rational design of nanomaterials
- Open weekly working meetings; members are from over 20 organizations--academia, government, industry, U.S./International
 - NIH, EPA, NIST, FDA, CDC, NIOSH
 - Stanford, Duke, UCLA, UNC, Oregon State, MSKCC, University of Birmingham, etc.
 - Alliance for Nanotechnology in Cancer, NNI, National Nanomanufacturing Network, EU NanoSafety Cluster, etc.
 - Pennsylvania NanoSystems, R&R Data Services, etc.

<https://nciphub.org/groups/nanowg>

Stacey Harper, PhD
Oregon State



Christine Hendren, PhD
Duke University
CEINT



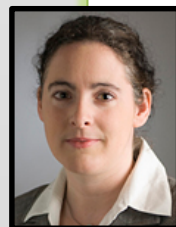
NIH > NATIONAL CANCER INSTITUTE



Center for Biomedical
Informatics and
Information
Technology



National Cancer Informatics Program



Iseult Lynch, PhD, MBA
University of Birmingham

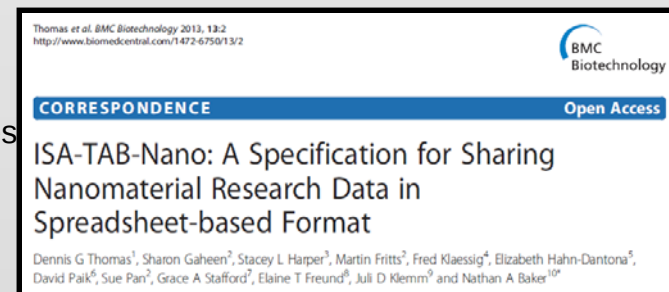
Nanotechnology
Working Group



Luisa Russell, PhD
NCI/NIH

Evolving Goals of the NCIP Nano WG

- Maintain the focus on concerted efforts in nanoinformatics in nanomedicine and nanomaterial development
 - Renewed focus on nanomedicine efforts; including QSAR-related research
- Bridging nanomedicine and nanotoxicology (NanoEHS)
 - Much to learn from each other, not just from an informatics perspective
 - Acknowledge individual needs of each field; presentations from both groups to facilitate interactions
- Synergize efforts in nanoinformatics across the US and EU
 - Catalogue of existing databases and tools to enable global collaboration
 - Continued development and expansion of the NPO and ISA-TAB Nano data exchange format
 - ISA-TAB-Nano has been adopted and adapted by the broader community
 - Extending files for functional assay and mammalian toxicity templates
 - Developing Wikipedia article on Nanoinformatics—led by Egon Willighagen (Maastricht, eNanoMapper) and John Sadowski (NIOSH, Wikipedian-In-Residence)
 - Build a community of practice around nano-data collection, re-use, metadata requirements, and integration (Nanomaterial Data Curation Initiative)



Nanomaterial Data Curation Initiative (NDCI)

Purpose:

- Capture a snapshot of current curation practices and concerns
- Develop recommendations for moving toward increasingly harmonized curation practices

Subtopic Areas	Description	
Framing Paper	Identifying stakeholders, Introducing strategy to take a snapshot of current nanoinformatics field, recommendations for integrated curation approach. Beilstein J. Nanotechnol. 2015, 6, 1752-1762	 BEILSTEIN JOURNAL OF NANOTECHNOLOGY 2015, 6, 1752-1762. The Nanomaterial Data Curation Initiative: A collaborative approach to assessing, evaluating, and advancing the state of the field Christine Ogilvie Hendren ^{*1} , Christina M. Powers ^{2,3} , Mark D. Hoover ⁴ and Stacey L. Harper ^{5,6}
Curation workflows	Capture the current processes in nanomaterial data curation. Beilstein J. Nanotechnol. 2015, 6, 1860-1871	 BEILSTEIN JOURNAL OF NANOTECHNOLOGY 2015, 6, 1860-1871. Nanocuration workflows: Establishing best practices for identifying, inputting, and sharing data to inform decisions on nanomaterials Christina M. Powers ^{1,2} , Karmann A. Mills ³ , Stephanie A. Morris ⁴ , Fred Klaessig ⁵ , Sharon Gaheen ⁶ , Nastassja Lewinski ⁷ and Christine Ogilvie Hendren ^{*8}
Data completeness and quality	Addresses the level and quality of data needed to meet scientific objectives. Nanoscale 2016, 8, 9919-9943	 2016, 8, 9919-9943. Nanoscale FEATURE ARTICLE View Article Online View Journal View Issue  Cite this: <i>Nanoscale</i> , 2016, 8, 9919 How should the completeness and quality of curated nanomaterial data be evaluated? [†] Richard L. Marchese Robinson, ^a Iseult Lynch, ^b Willie Reijnenburg, ^{c,d} John Rumble, ^e Fred Klaessig, ^f Clarissa Marquardt, ^g Hubert Rauscher, ^h Tomasz Puzyn, ⁱ Ronit Purian, ^j Christoffer Åberg, ^k Sandra Karcher, ^l Hanne Vriens, ^m Peter Hoet, ⁿ Mark D. Hoover, ^o
Curator responsibilities	Established and developing roles in the curation process; challenges associated with quantity vs. quality of data entries. Manuscript in preparation.	
Data Integration	How do we define and operationalize integration between databases and datasets? NanoImpact 2018, 9, 85-101	
Metadata	How an instance of characterization is represented to enable comparisons and reproducibility. Manuscript in preparation	Research paper NanoImpact 2018, 9, 85-101. Integration among databases and data sets to support productive nanotechnology: Challenges and recommendations Sandra Karcher ^{a,q} , Egon L. Willighagen ^b , John Rumble ^{c,d} , Friederike Ehrhart ^b , Chris T. Evelo ^b , Martin Fritts ^e , Sharon Gaheen ^e , Stacey L. Harper ^f , Mark D. Hoover ^g , Nina Jeliaskova ^h , Nastassja Lewinski ⁱ , Richard L. Marchese Robinson ^{j,k,l,1,2} , Karmann C. Mills ^l , Axel P. Mustad ^m , Dennis G. Thomas ⁿ , Georgia Tsiliki ^{o,p} , Christine Ogilvie Hendren ^{q,*}

nciphub.org/groups/nanotechnologydatacurationinterestgroup

Thrust 2—Foster an Agile Modeling Network

An **agile modeling network** for multidisciplinary intellectual collaboration that effectively couples experimental basic research, modeling, and applications development

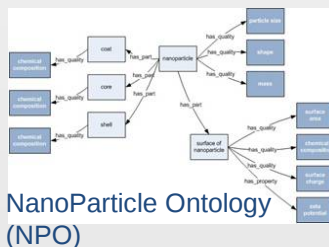
- NKI agencies are contributing to the development of computational models and modeling tools
- Example modeling resources include those supported by NSF:
 - **nanoHUB**—virtual platform for computational nanotechnology research, education, and collaboration; hosts over 320 simulation tools
 - **Knowledgebase of Interatomic Models (KIM)**—online suite of open source tools for molecular simulation of materials

Thrust 3—Build a Sustainable Cyber Toolbox

A **sustainable cyber-toolbox** to enable effective application of models and knowledge to nanomaterials design

nanoHUB.org

**NANOPARTICLE
INFORMATION
LIBRARY**



GoodNanoGuide

ClinicalTrials.gov
A service of the U.S. National Institutes of Health

NCIP | HUB

National Cancer Informatics Program
Nanotechnology Working Group

nanoinfo

caNanoLab

InterNano
Resources for Nanomanufacturing

ToxCast™

**International Clinical Trials
Registry Platform
Search Portal**

NANOMATERIALREGISTRY

**MATERIALS
PROJECT**

**NBI
KNOWLEDGEBASE**

XSEDE
Extreme Science and Engineering
Discovery Environment

<http://www.nano.gov/NKIPortal/CyberToolbox>

Thrust 4—Create a Robust Digital Nanotechnology Data and Information Infrastructure

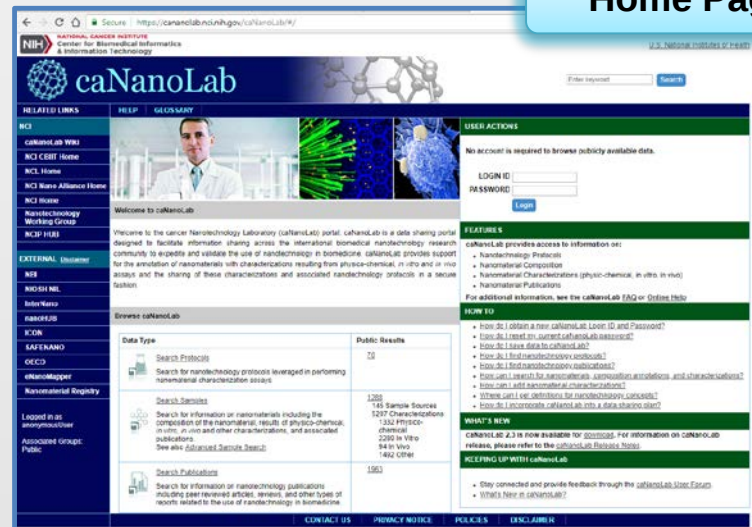
- A robust digital nanotechnology data and information infrastructure to support effective data sharing, collaboration, and innovation across disciplines and applications. Efforts include:
 - Vetting existing and emerging nanotechnology data and information using standardized formats and vocabulary
 - Data Readiness Levels (<http://www.nano.gov/NKIPortal/DRLs>)—organized by NKI members and is analogous to technology readiness levels; shorthand method of communicating data maturity and quality to support informed data sharing.
 - Providing the broader research community with access to reliable data and protocols
 - NIOSH's GoodNanoGuide—online-based collaboration platform; forum for up to date info and current good practices for managing nanomaterials in a work-related environment
 - NIH's caNanoLab and Nanomaterial Registry

caNanoLab Data Portal: A Resource for Data Sharing

caNanoLab Goal

To provide a nanotechnology resource that facilitates data sharing in the community to expedite and validate the use of nanomaterials in biomedicine

Home Page



<https://cananolab.nci.nih.gov/caNanoLab/>

- Provides access to samples, protocols, and publications from the NCI Nanotechnology Characterization Laboratory (NCL), NCI Alliance for Nanotechnology in Cancer, and the broader biomedical nanotechnology community
- Provides support for the annotation of nanomaterials with composition information, and physico-chemical, *in vitro*, and *in vivo* characterizations
- Launched 2006—in-house data curation; 2015—Alliance data coordinators
- Over past few years new collaborations with other databases and research programs

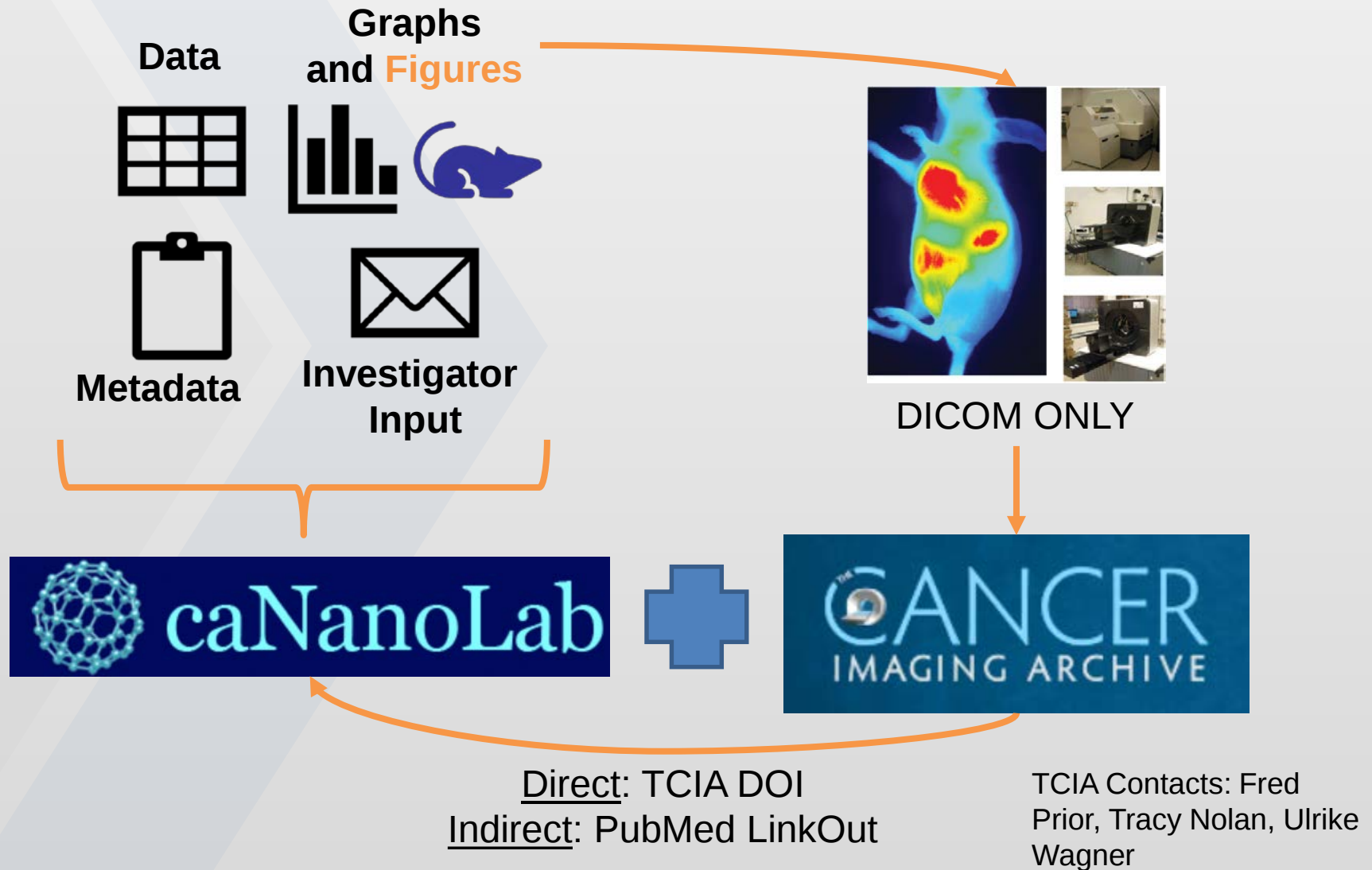
- Data submission a term and condition of award
- Alliance Data Coordinators are responsible for coordinating submission of nanomaterial characterizations, protocols, and publications associated with funded awards
- caNanoLab activities *must* be reported in annual reports

CCNE (U54s)	Data Coordinator
Caltech/UCLA/ISB	Wei Wei Dana Levine (Project 1)
Northwestern	Gokay Yamankurt (Project 3) Eric Berns (Project 1) Serena Ghelfi (Project 2) Robert Molto Pallares (Core)
Stanford	Alice Fan Thomas Metzner
UNC-Chapel Hill	Marina Sokolsky Mingzhen Zhang Duhyeong Hwang
Washington U	Malcolm Tobias Fred Prior Tracy Nolan
MSKCC/Cornell	Luis Campodonico

CNTCs (T32s)	
MD Anderson/Rice	Stacey Kalovidouris

IRCN (U01s)	Data Coordinator
Case Western (Karathanasis)	Ketan Ghaghada
UCLA (Tseng)	Matthew Smalley
UNC-Chapel Hill (Kabanov)	Marina Sokolsky
Emory (Yang)	Tongrui Liu
UC Davis (Lam)	Wenwu Xiao Yuanpei Li
UCLA (Nel)	Huan Meng Xiangsheng Liu
U of Chicago (Lin)	Kaiyuan Ni
Ohio State (Guo)	Daniel Binzel
Masimo (Lapotko)	Katsiaryna Hleb
MGH (Weissleder)	Miles Miller
University of Texas MD Anderson Cancer Center (Lopez-Berestein)	Pinar Kanlikilicer
UCSD (Steinmetz)	Sourabh Shukla
Iowa State (Narasimhan)	Kathleen Ross
UT Southwestern (Gao)	Zhaohui Wang

In Progress: caNanoLab Integration with The Cancer Imaging Archive



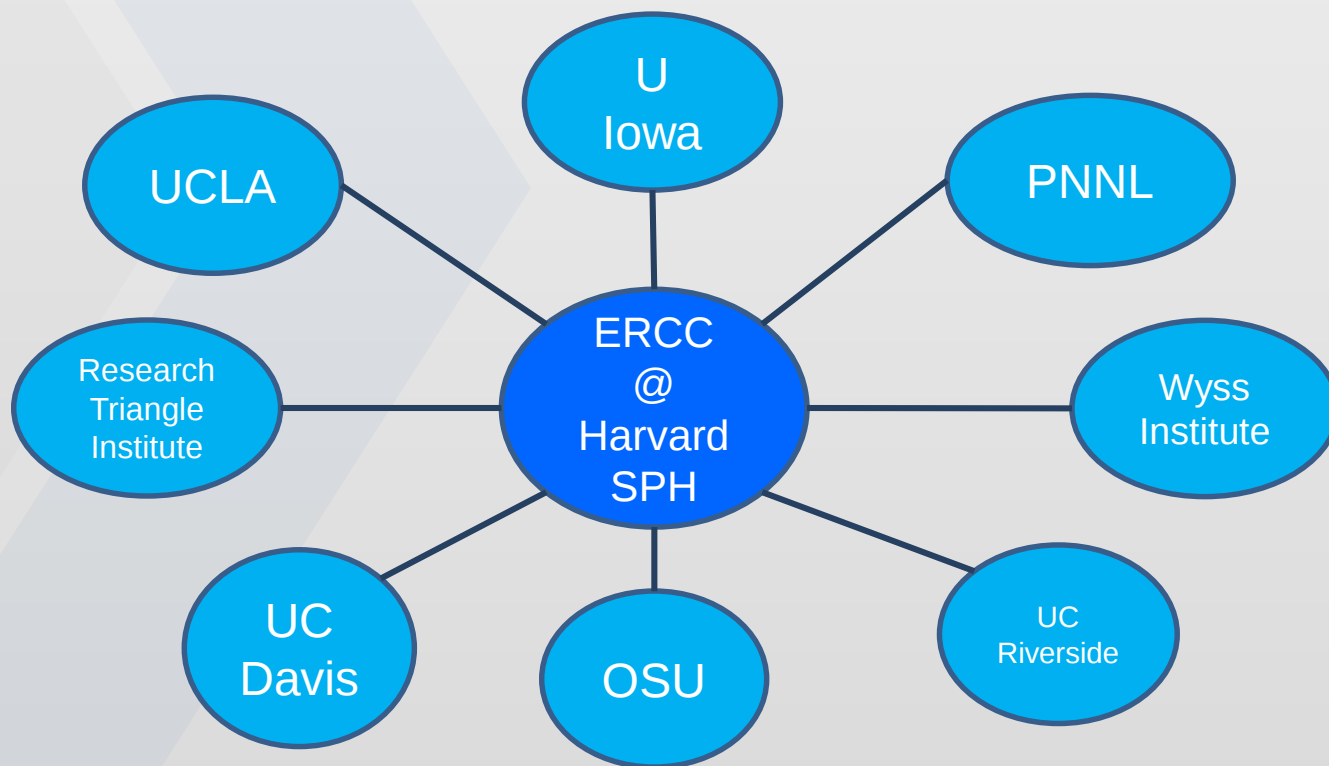
Nanotechnology Health Implications Research Consortium



National Institute of Environmental Health Sciences
Your Environment. Your Health.

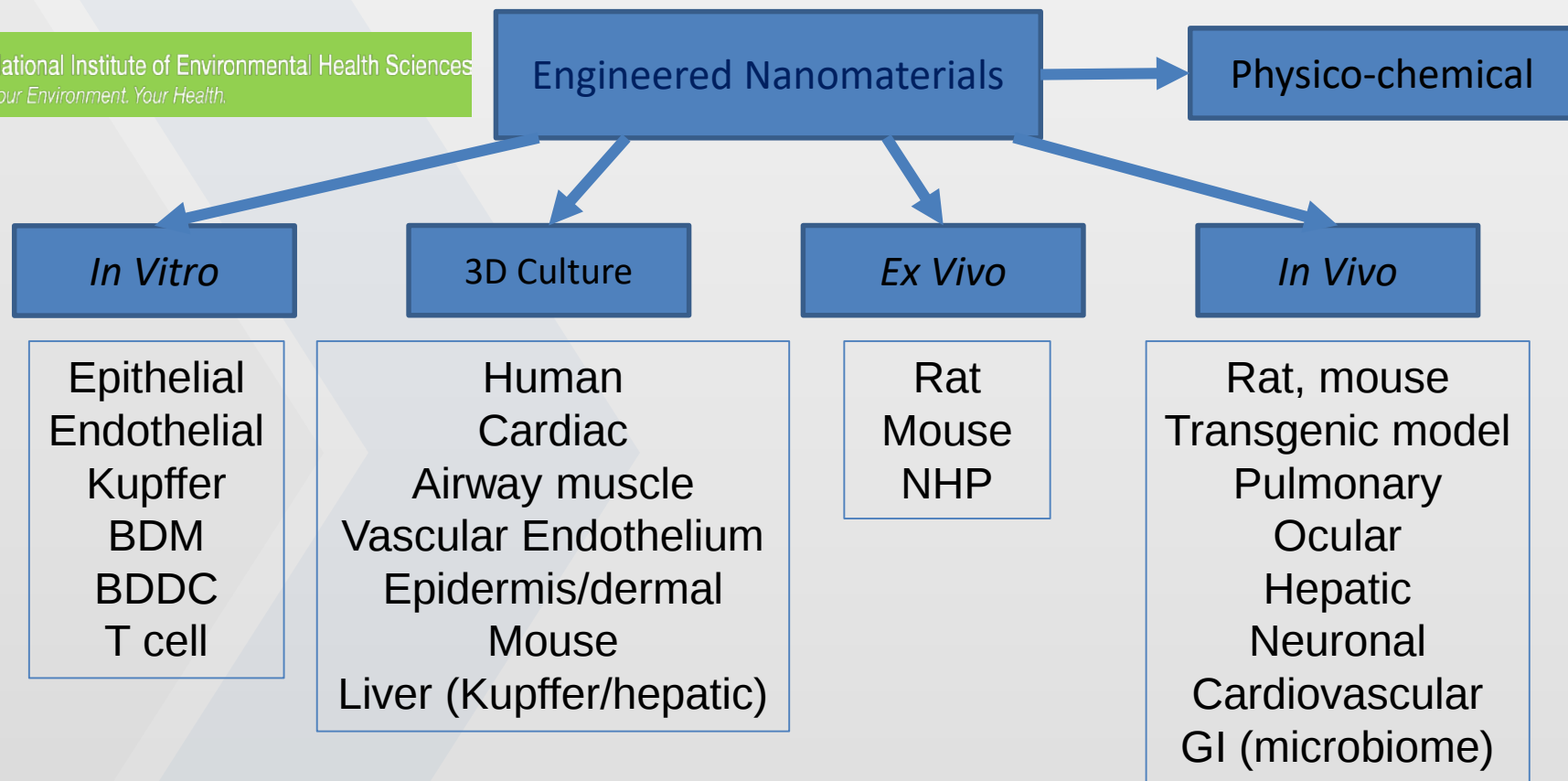
Nanotechnology Health
Implications Research
Consortium (2016-2021)

NHIR Consortium



ERCC: Engineered Nanomaterials Resource and Coordination Core

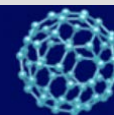
Nanotechnology Health Implications Research Consortium



Biological Response Profiles

NP Types: metals, metal oxides, carbon nanotubes, 2-D and 3-D engineered nanomaterials, metal-metal conjugates, and cellulose

Future Modeling Efforts



caNanoLab

Submitted: 23 Protocols

24 Publications 24 Samples

Proposed and Upcoming New caNanoLab Features

- Refocus of curation efforts to improve usability
 - Increased uniformity of entries across project sites; streamlining dropdown menus
 - Increased speed of submission (submission template forms and work on submission through eNanobook (supplemented Alliance project))
- Assigning DOIs to complete data sets in caNanoLab
 - DataCite through CBIIT/NCIPHub
- Collecting input to build a caNanoLab API
- Introducing a new section on Nanomaterials Synthesis
- Expanded social media presence-- #caNanoLab
 - Further exposure for those who submit and reaching a wider audience of submitters
- **NCIcaNanoLab@mail.nih.gov**

Acknowledgements

Piotr Grodzinski

Christina Liu

Christopher Hartshorn

Luisa Russell

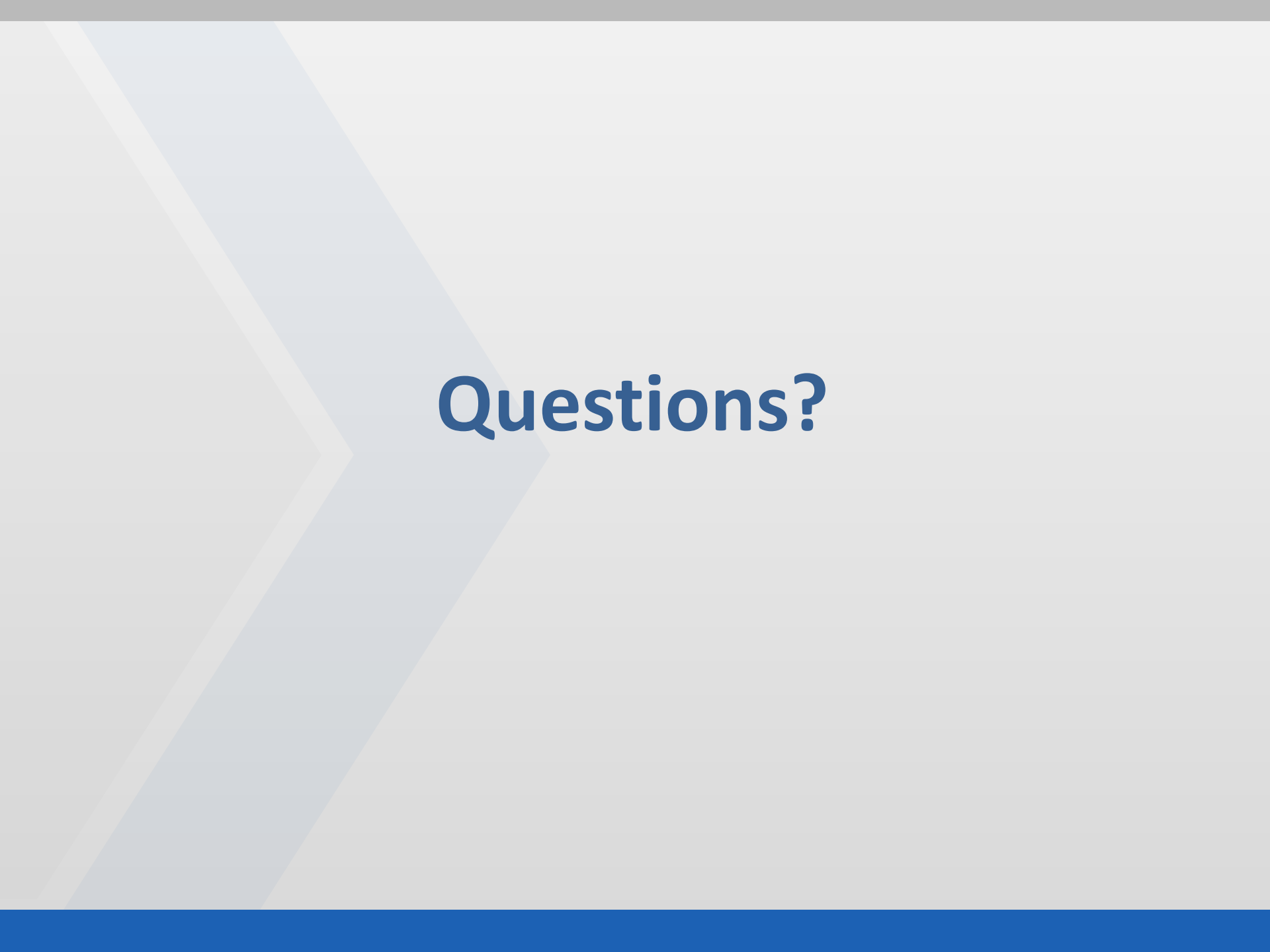
Mervi Heiskanen

Philippa Barnes

Michal Lijowski

NKI

NCIP Nano WG



Questions?