NNI Nanoinformatics Conference: November 15, 2023

On November 15, 2023, the NNI held its first Nanoinformatics Conference, which was co-hosted by the NNCO, on behalf of the NNI, and the INFRAMES project. As nanotechnology has progressed over the years, it has become clear that there was a need to adapt and develop informatics tools and methods to capture the complex and dynamic nature of nanoscale phenomena. Nanoinformatics is thus the use of informatics techniques to analyze and process information about nanomaterials' structures and applications, as well as their characteristics, behaviors, and transformations. While this need was addressed in the NNI's 2011 NNI Environmental, Health, and Safety Research Strategy, since its publication, advances in informatics and the ubiquity of nano-enabled technologies increased the need to support the NNI's nanoinformatics infrastructure and to foster greater connections among the nanoinformatics, nanosafety, and broader informatics communities.

The NNI placed significant emphasis on international participation in the event, holding the meeting adjacent to the 2023 U.S.-EU NanoEHS Communities of Research (CORs) Workshop. The in-person-only conference attracted more than 40 attendees from the United States, Europe, Asia, and Latin America, representing academia, state and local governments, industry, as well as the Federal government. Visit the Conference webpage for additional information on the meeting agenda and speakers.

The NNI has historically supported the growth of a vibrant and multidisciplinary international community engaged in diverse activities and forums. The positive public response to the event indicates interest in contributing to these efforts. NNCO sought community involvement early on in planning the meeting and shared coordinating responsibilities with U.S. EPA (EPA) representatives on the Federal interagency databases informal interest group (DIIG) and INFRAMES collaborators at Duke University.

NNCO Deputy Director Quinn Spadola welcomed attendees and introduced conference co-organizers and conference co-chairs Holly Mortensen (EPA) and Jaleesia Amos (Duke University). The opening speaker at the conference was environmental and molecular toxicologist Stacey Harper, from Oregon State University. Harper described the ways informatics improves daily life and public services, fostering innovation, efficiency, and interdisciplinary collaborations. She noted that predictive toxicology remains an important goal for nanosafety scientists and is facilitated today by a greater capacity to harness the power of information systems.

The conference's keynote speaker, Christopher S. Marcum, of the White House Office of Management and Budget, spoke about the Year of Open Science, which was announced by the White House in January 2023. Marcum described the importance of open science to the nation's taxpayer-supported research and innovation enterprise. Noting that public access is not synonymous with open access, Marcum gave examples of activities undertaken by Federal agencies to improve public access to science, as well as U.S. bilateral efforts in this area. Attendees posed a wide range of questions to Harper and Marcum on the peer-review process and data reproducibility, and how to navigate contrasting data access and privacy policies across national and regional jurisdictions. The discussion also explored workable incentives for storage, access, and retrieval of data across agencies and domains.

The remainder of the morning session focused on progress and next steps for the U.S. and EU nanoinformatics community. Presentations by EU nanoinformaticists and nanosafety experts highlighted the role of nanoinformatics in creating Findable, Accessible, Interoperable, and Reusable (FAIR) data

standards and in nanomaterial safety and sustainability. From the U.S. perspective, key investments include the NIH's CaNanoLab, which is a cancer nanotechnology data-sharing portal. Also, updates on DIIG's effort to build an interagency consortium to make Federal nanosafety databases interoperable and more accessible were shared.

By the end of the morning session, it became clear from the presentations that progress in many areas of nanoinformatics and chemoinformatics has involved close collaboration between the U.S. and EU communities, the publication of the EU-US Roadmap Nanoinformatics 2030 being a landmark example of U.S.-EU cooperation. Another good example of such collaborative efforts is joint work by U.S. and EU researchers, as well as other groups, to close the gap in informatics and modeling needs for robust nanotechnology risk assessment. Progress in this area includes the use of semantic web approaches to make EPA's Adverse Outcome Pathways Database interoperable with the AOP Wiki database. EPA has used this approach to create interoperable file formats for the nanomaterials database NanoKnowBase. Conference presenters also spoke about lessons from inter-laboratory studies, the use of semantic web applications to make databases interoperable, and the creation of a machine-readable nanomaterial-specific International Chemical Identifier (NInChI). NInChI would create a simplified machine-readable representation of complex nanomaterials across experimental and nanoinformatics studies.

Knowledge and the associated data infrastructure are key elements of a healthy global nanotechnology research ecosystem. A significant portion of the Conference agenda was dedicated to next steps. Among the takeaways was the importance of advancements and evolution in certain areas: standardization and automatization of data collection and management for FAIR data; standards within nanotechnology for consistent metadata; data longevity and sustainability of informatics platforms; and the need to adapt databases and tools with changes within nanotechnology and the community. Training and workforce development were cited as key components in increasing the use and reuse of academic data and in building a greater understanding of how regulators use and reconfigure data. In closing remarks, conference co-host Jaleesia Amos told attendees that "based on discussions today, there is strong energy in this community and significant support for bringing together the nanotechnology and informatics communities." The NNI is grateful for the perspectives and ideas provided by participants and their continued energy in broadening and strengthening the nanoinformatics community.