

Accelerating Adoption of NAMs with FAIR Principles S Bell¹, P Ceger¹, J Fostel², S Holmgren², AM Masci², DG Allen¹, W Casey², N Kleinstreuer³ ¹ILS, RTP, NC, USA; ²NIH/NIEHS/DNTP, RTP, NC, USA; ³NIH/NIEHS/DNTP/NICEATM, RTP, NC, USA

Highlights

- Data obtained using new approach methodologies (NAMs), particularly in vitro assays, require additional context to link to in vivo toxicity endpoints
- NIEHS and the National Toxicology Program (NTP) support adoption of knowledge organization systems and FAIR data principles to further scientific advancement in environmental health sciences
- Improving the FAIRness of data is critical for providing data context and enabling the information integration needed for assessment, interpretation, and method development
- Examples from two NTP resources exemplify the value of using structured knowledge organization to support FAIR data principles.

What are FAIR data principles?

Findable

• Data is findable by people and machines using unique and persistent IDs accompanied by rich metadata

Accessible

• (Meta)data are accessible in an open and standardized format

Interoperable

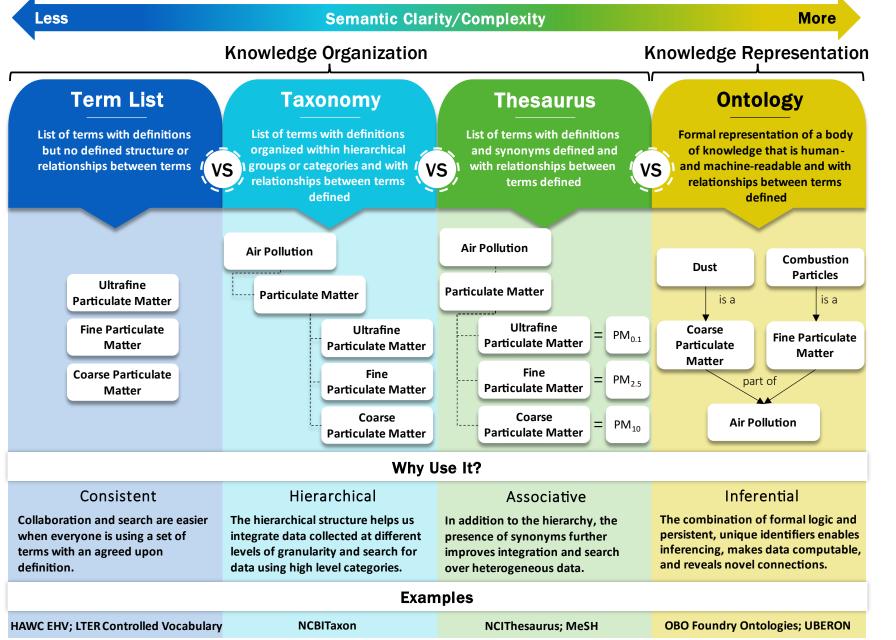
• A formal, broadly applicable knowledge organization system is used to describe (meta)data and relationships

Reusable

(Meta)data are well described to promote integration with other resources

Annotation of data to support FAIR

Data annotation using knowledge organization impart standardization and structure needed to achieve data FAIRness



- Increased tools and education to support adoption
- Reporting requirements by journals and funding agencies

commentary available:

https://www.mdpi.com/1660-4601/18/17/8985

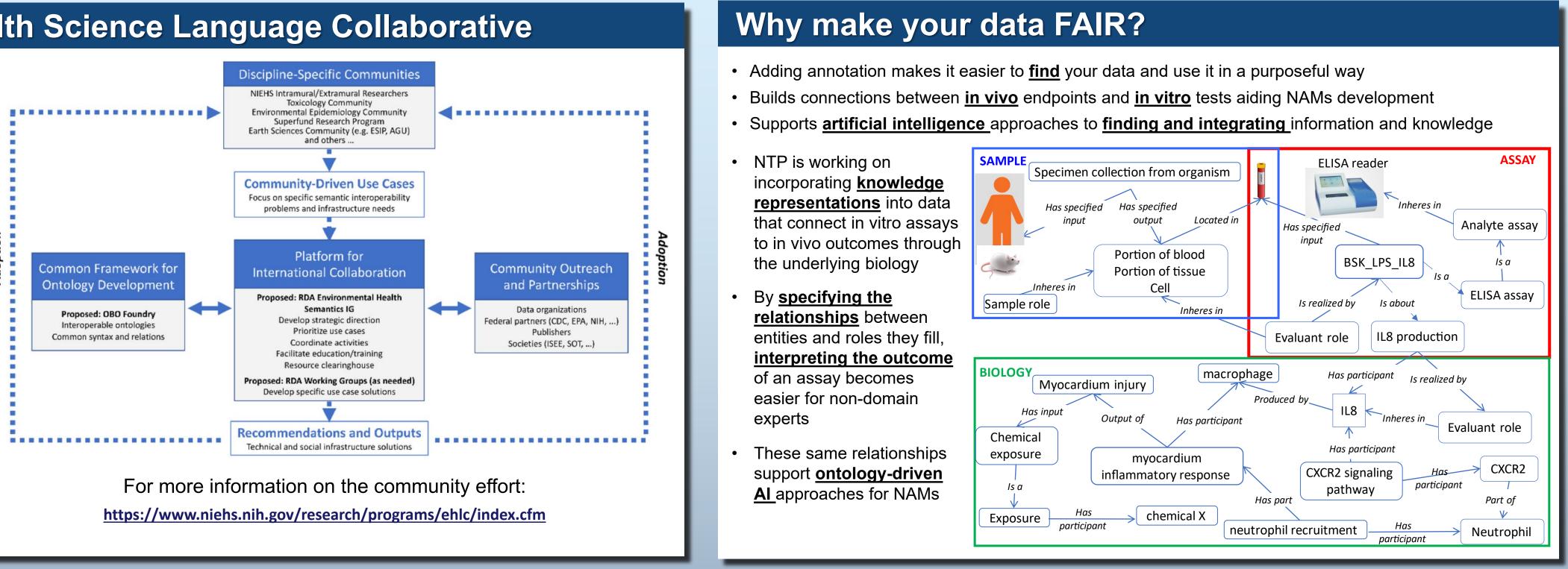
What do FAIR principles look like in a data repository? • The NTP's Chemical Effects in Biological Systems (CEBS) is a comprehensive and unique toxicology resource containing individual and summary in vivo and in vitro data from NTP and other depositors • Annotation of study information using knowledge organization systems in CEBS improves accessibility and **interoperability** of data **Ongoing efforts supporting FAIR data** Study Metadata Conclusions Study Data within CEBS Continued harmonization and annotation In-life Data Study Conclusions of new and legacy datasets Trial Results ithor Study curation using the OBO foundry In Vivo and In Vitro Data: etc. Statistical Results Histopathology family of interoperable ontologies means iroup **Clinical Pathology** Activity Calls study data is reusable Toxicogenomics Immunology Development of tools to improve and Fold Changes PCR expand search functionalities of detailed Genetic Toxicology, etc study information improves the ability of eristics users to **find** desired information Microarray Data High-throughput Data Use of standardized terminology DOSE allows for data to be integrated across multiple studies to facilitate study VEHICLE integration and allows for additional knowledge discovery STRUCTURA https://cebs.niehs.nih.gov/cebs/ GROUP

Study Details Title
Contributing Au Study Factors,
Experimental G
Subjects
Protocol
Subject Characte
Timeline

Environmental Health Science Language Collaborative

National Institute of Environmental Health Sciences (NIEHS) sponsored a September 2021 virtual workshop focused on **building a** sustainable community and developing sustainable semantic solutions to support the advancement and adoption of harmonized environmental health language approaches

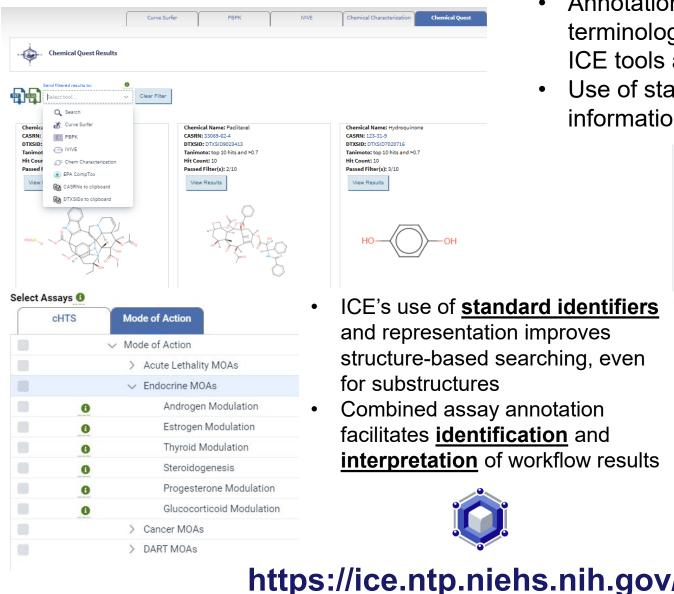
- Participants identified a need for:
- Workshop report describing the needs and outcomes forth coming; preworkshop



Improving access to NAM data and tools using FAIR

- The NTP's Integrated Chemical Environment (ICE) provides stakeholders access to data and tools supporting NAMs
- ICE relies on curation by domain experts to improve the **findability** of data for diverse users and the accessibility of the data from ICE tools • Annotation of mechanistic in vitro assays to standardized

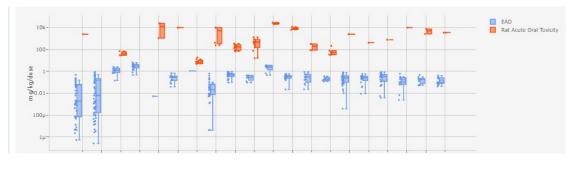
ICE tools and beyond



Chemical Name: Hydroquinone
CASRN: 123-31-9
DTXSID: DTXSID7020716
Tanimoto: top 10 hits and ≻0.7
Hit Count: 10
Passed Filter(s): 3/10
View Results
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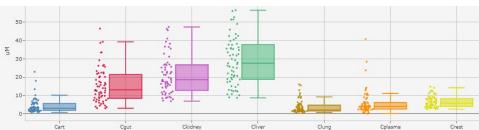
• ICE's use of standard identifiers and representation improves structure-based searching, even for substructures Combined assay annotation facilitates **identification** and interpretation of workflow results





information outside of ICE, including with CEBS

ICE's annotations combined with ICE's browser-based workflows support NAMs by aiding in *identifying* relevant assay and chemical data needed to support read across in vitro to in vivo comparisons (above), and tissue-level chemical distribution (below)



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