WorldFAIR

SPRING 2023

IUPAC

Division of Chemical Information

IUPAC WORKSHOP

ADVANCING FAIR CHEMISTRY: DEVELOPING NEW SERVICES FOR SHARING CHEMICAL DATA

March 27, 2023, Indianapolis
In-person & Hybrid

Workshop Brief Summary: Advancing FAIR Chemistry: Developing New Services for Sharing Chemical Data

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March 27, 2023. ACS Spring Meeting. Indianapolis. USA
Organizers: Leah McEwen, Ian Bruno, Stuart Chalk, Evan Bolton, and Fatima Mustafa

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1. **Speakers**
   - Cornell University: Leah McEwen
   - Cambridge Crystallographic Data Center: Ian Bruno
   - University of North Florida: Stuart Chalk
   - U.S. National Center for Bioinformatics: Evan Bolton
   - St. Olaf College: Robert Hanson
   - University of Alabama: Vincent Scalfani
   - IUPAC: Fatima Mustafa

2. **Summary**

The goal of WorldFAIR* Chemistry is to support the use of chemical data standards in research workflows to enable downstream data reuse through practical direction and resources. The aim of this workshop was to engage the input and expertise of stakeholders across the chemistry community on prototype services and other IUPAC standards activities in progress. We presented early work on each of these resources and invited the community to share feedback on what will help them to implement these in your workflows - What works well? What needs further refinement? What is missing?

WorldFAIR Chemistry prototype deliverables:

- **Guidance** [1]: recommendations for managing and sharing FAIR chemical data for various stakeholders.
- **Cookbook** [2]: recipes (Cookbook) for preparing and depositing FAIR machine-enabled chemical data.
- **Protocols** [3]: universal protocol for browser-based validation and lookup services

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[1] https://iupac.org/project/2022-027-1-024
[2] https://iupac.org/project/2022-028-1-024
[3] https://iupac.org/project/2022-029-1-024

IUPAC standards projects:

- **Doc-a-thon: Chemical representation best practices for humans and machines**. This session focused on reviewing the existing IUPAC graphical representation standards for chemical structure diagrams and stereochemical representation with considerations for machine-readability.

- **IUPAC FAIRSpec[4]-ready aggregations: Recommendations for researchers, authors, and publishers.** IUPAC is developing specifications for aggregating spectroscopy data and chemical structures for reporting spectroscopy measurements. The resulting data collections can be created either manually by a researcher or automatically by an electronic laboratory notebook (ELN) or laboratory instrument management system (LIMS) and the accompanying metadata can also be used as a finding aid.

3. Key discussion points

1. Ideally, data management resources should be capturing metadata from the point of sample identification, experimental techniques, data collection, measurement parameters (including units), instruments, analysis, etc. through publication and re-use.
2. IUPAC standards need models for digital representation, including chemical systems, quantities, measurements and criteria for interoperability.
3. Ambiguity may not always be apparent until formats are moved from system to system, round-trip testing can help with review of specifications.
4. Consider data curators and others managing data who don't necessarily have extensive domain knowledge.

[4] https://iupac.org/project/2019-031-1-024