IUPAC FAIR Chemistry Cookbook

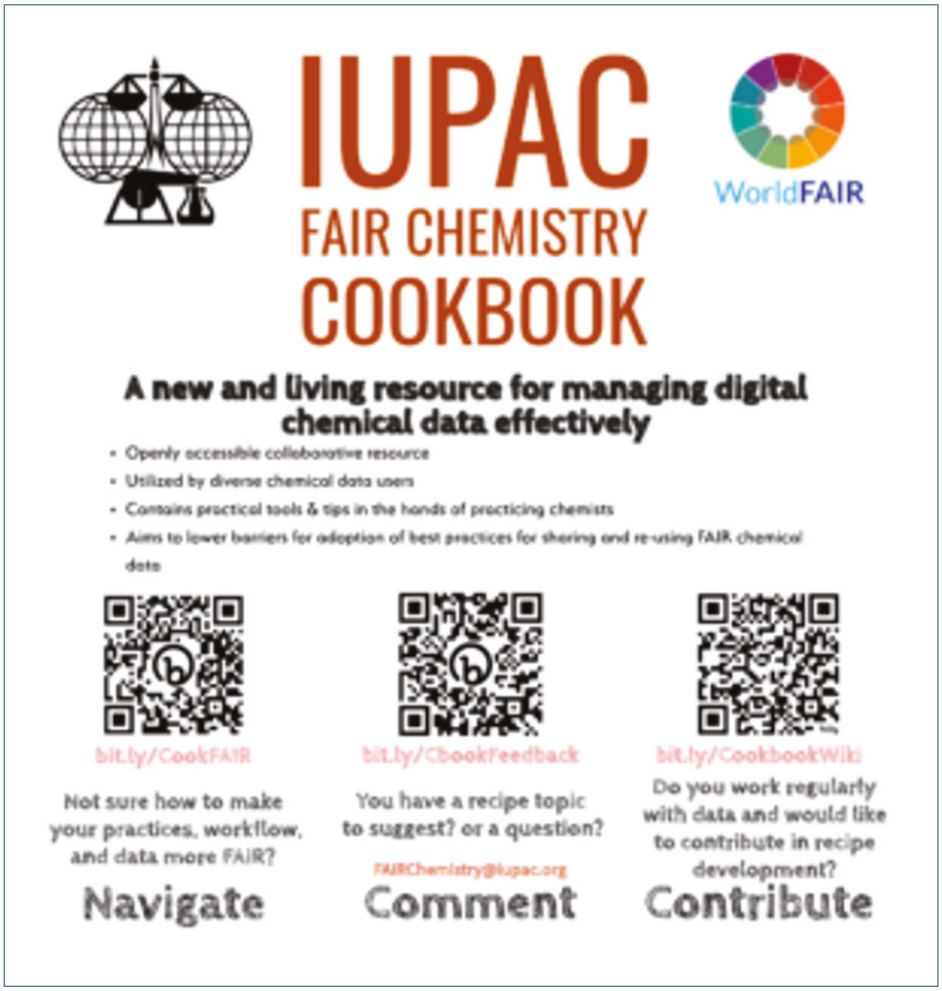
The IUPAC FAIR Chemistry Cookbook is a new living resource developed to enable the chemical sciences community to move toward sharing and reusing data, code, metadata, *etc.* **that are *F**indable, **A**ccessible, **I**nteroperable, and **R**eusable* or ***FAIR*.**

Chemistry underlies both living and materials systems and chemical data are at the heart of data driven discovery and innovation across the health and environmental science sectors and in many applied engineering fields. Chemical data and analysis tools are increasingly available online and researchers and practitioners alike are increasingly involved in new ways to analyze, visualize, mine, and integrate data and information.

In a digital work environment, well-prepared researchers need to be comfortable working their way around digital data formats, code, and online computing platforms. Proficiency in basic digital data handling skills can empower chemists to exploit FAIR and open data resources and handle real-world chemical data scenarios more effectively. As a result, the **Cookbook** content is designed to train, encourage, and enable chemistry researchers and data professionals to help support practices, workflows and data that are more FAIR.

Cookbook highlights

- **Practical Training Materials**: Developed by active members to demonstrate protocols for managing machine-readable chemical data.
- **Scope**: Recipes cover a wide range of tasks and use cases for handling chemical data programmatically.
- **FAIR Principles**: Emphasizes data being Findable, Accessible, Interoperable, and Reusable, aligned with FAIR machine-readable data criteria.



- **Educational Focus**: Supports learning for researchers and students on navigating diverse data types, extracting insights programmatically, and applying automated approaches for curation, dissemination, and analysis.
- **Interactive Tutorials**: Provides hands-on experience with digital data sources, tools, and workflows, enhancing understanding through executable code blocks and common cheminformatics functions.
- **Community Repository**: Offers readily accessible online tutorials for users to engage with, exemplifying FAIR principles for data reuse.
- **Online Accessibility**: Easily accessible through existing online infrastructure, facilitating widespread use and adoption.

How to use the Cookbook

This cookbook provides a range of protocols developed by active community members. These recipes target different tasks across a range of possible use cases for working with machine-readable chemical data (*i.e.*, FAIR data). The cookbook presents a collection of annotated code snippets and workflows for specific tasks in manipulating machine-readable chemical data and metadata.

- **Jupyter Notebooks:** Many of the recipes on this site take advantage of Jupyter Notebooks to run Python code in the browser for an interactive (and educational) feel for the user.
- **When is a recipe useful and for what?** Info is available in the collapsable 'header' below the title of the recipe. Header: also includes bullets for skills and learning objectives
- **Ideas to further characterize the applicability of recipes?** Ideas are welcome

Contribute to the Cookbook!

If you regularly work with digital chemical data and have useful approaches that could be demonstrated through a Jupyter Notebook, please consider contributing. Best practices for using standards and tools are emphasized and instructions for how to contribute materials are provided.

Unlock Exclusive Benefits as a Contributor to the Cookbook:

- Gain Recognition: Your contributions will be acknowledged on the Cookbook's contributions page.
- Boost Your Profile: Your ORCID will be integrated into the metadata of your contributions.
- Secure Your Work Identity: Each contribution receives a unique ID through http://w3id.org, ensuring your work is properly attributed and easily accessible to others.

More information is available in Cookbook Wiki <https://bit.ly/CookbookWiki>
Contact: FAIRChemistry@iupac.org
https://iupac.org/iupac-fair-chemistry-cookbook/

In Memoriam—Allen Joseph Bard (1933–2024)

by Larry R. Faulkner and Christopher M. A. Brett

Professor Allen J. Bard, president of IUPAC during the biennium 1991-93, died in Austin at the age of 90 on February 11, 2024. He was a world-renowned electrochemist, recognized especially for placing the study of electrochemical reactions on a level of sophistication similar to that of homogeneous chemical processes.

In more than 60 years at the University of Texas at Austin, he guided 360 PhD students and post-doctoral associates and published more than 1000 peer-reviewed papers. The large topics on which he concentrated comprise a sizable fraction of electrochemistry in his time, including the mechanisms of electrode reactions, chemiluminescence from electrogenerated species, and photoelectrochemistry at semiconductor electrodes. He co-invented immunoassay by chemiluminescence and was an essential innovator in scanning electrochemical microscopy. Both tools have become commercially available and are widely employed. In his later years, he focused on what is now known as single-molecule electrochemistry, establishing methods that could detect individual electrochemical events. He often provided the first demonstrations. Some of his most striking results involved the formation and observation of individual catalytic centers of one to several atoms.

He is remembered as a superb teacher, able to inspire students through his own excitement with science and his ability to convey the essence of a complex subject with clarity and simplicity.

He also contributed through his influential texts, including three editions of *Electrochemical Methods* (Wiley, 1980, 2001, 2022, the last with L. R. Faulkner and H. S. White). Moreover, he edited three leading series in electrochemistry and was Editor-in-Chief of the *Journal of the American Chemical Society* for 20 years.