



IUPAC Committee on Publications and Cheminformatics Data Standards (CPCDS)

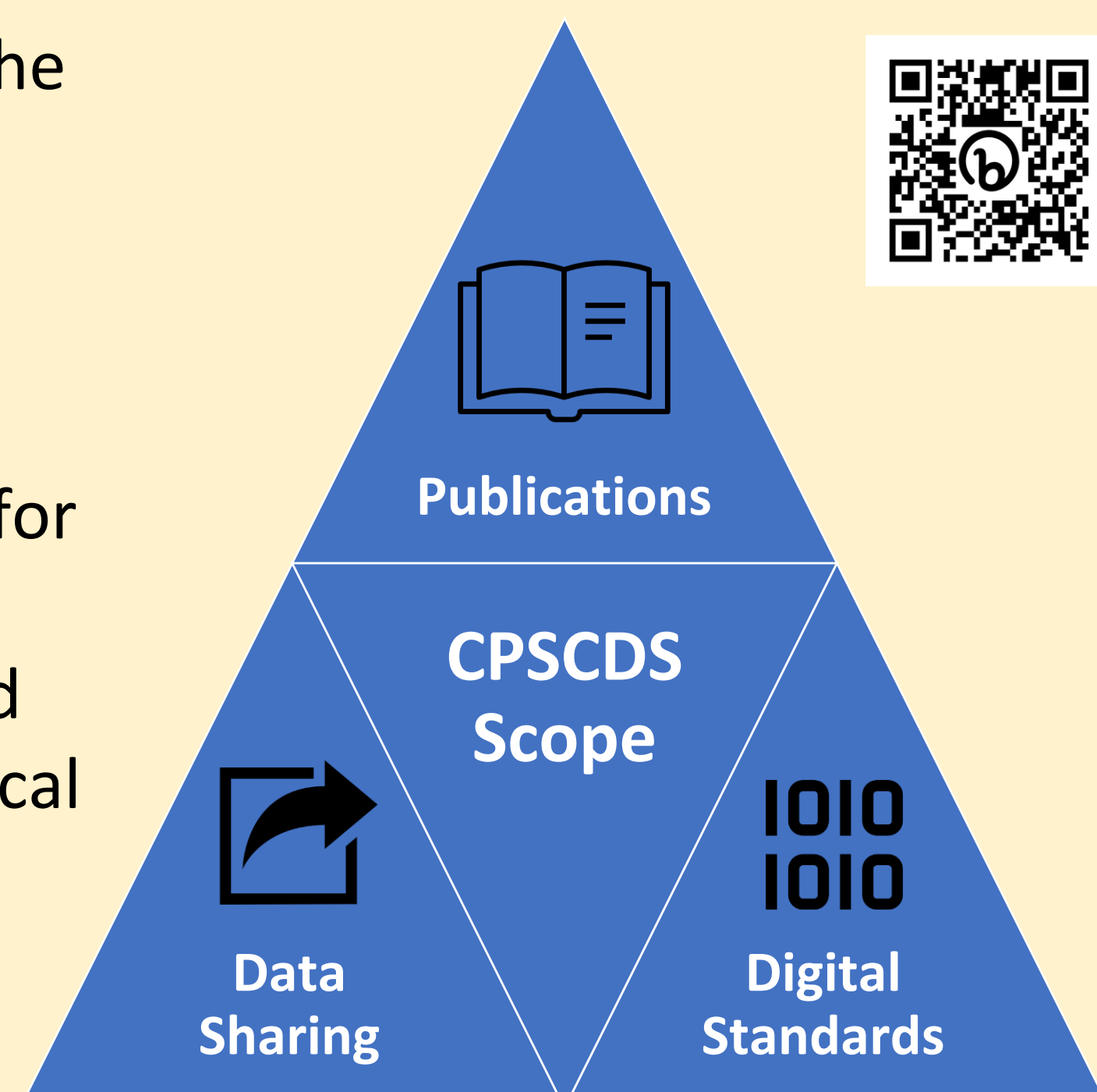
– Towards a Digital Era –

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SCOPE OF WORK

“This committee advises the Union on the design and implementation of **publications, data sharing and digital standards** development for promoting exchange and application of human and machine-readable chemical information.”



DIGITAL IUPAC

Communicating chemical knowledge is at the core of the IUPAC mission and underlies the success of the chemistry enterprise. In the global economy of the 21st century, this involves exchange among computer systems along with the expert scientists who use them. To enable the application of IUPAC expert standards in the digital environment, IUPAC must augment its efforts to enable accessibility and interpretation by machines as well as humans. The Union must adapt to a digital work culture to engage in its mission of sustainable development, common language and free exchange of scientific information.

IUPAC is strategically placed to collaborate broadly across the community to develop the tools and standards that will be needed by chemists and all those who use chemical data in the world of big data and to direct these collective efforts into Open Science and FAIR data initiatives globally and across disciplines.

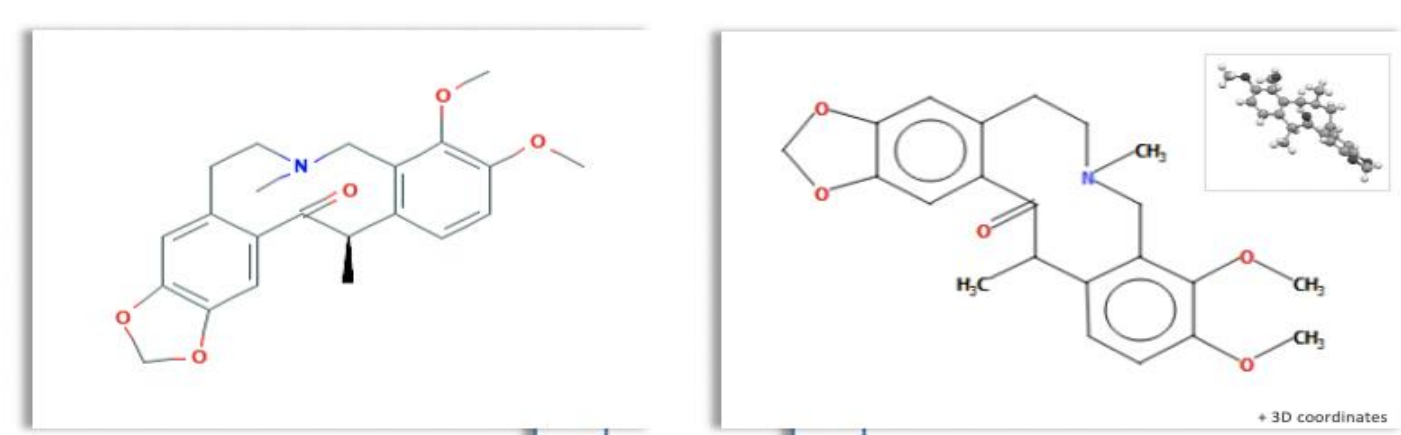
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PROJECTS & UPDATES

InChI

(IUPAC International Chemical Identifier)

InChI TRUST



Standard InChI:
InChI=1S/C22H25NO5/c1-13-15-5-6-18(25-3)22(26-4)17(15)11-23(2)8-7-14-9-19-20(28-12-27-19)10-16(14)21(13)24/h5-6,9-10,13H,7-8,11-12H2,1-4H3/t13-m/s1

Standard InChIKey: YRAXYCEEARNTF-ZDUSSCGKSA-N



Gold Book

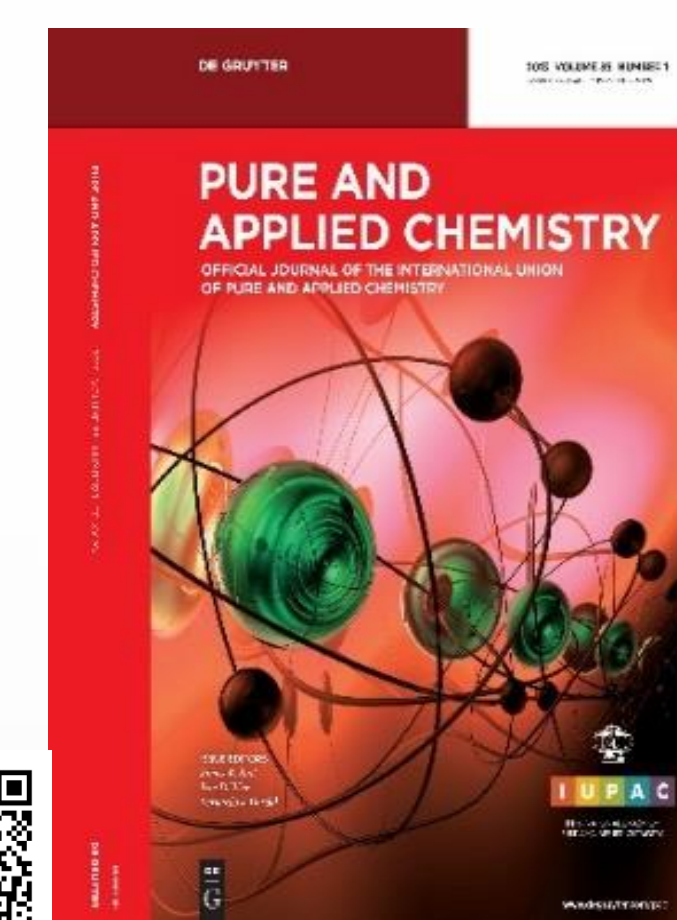
IUPAC Compendium of Chemical Terminology



Pure & Applied Chemistry

- IUPAC Recommendations & Technical Reports
- Authoritative lectures from at IUPAC conferences, symposia and workshops
- Special Topic Issues
- Cheminformatics Standards in Practice (call open)*

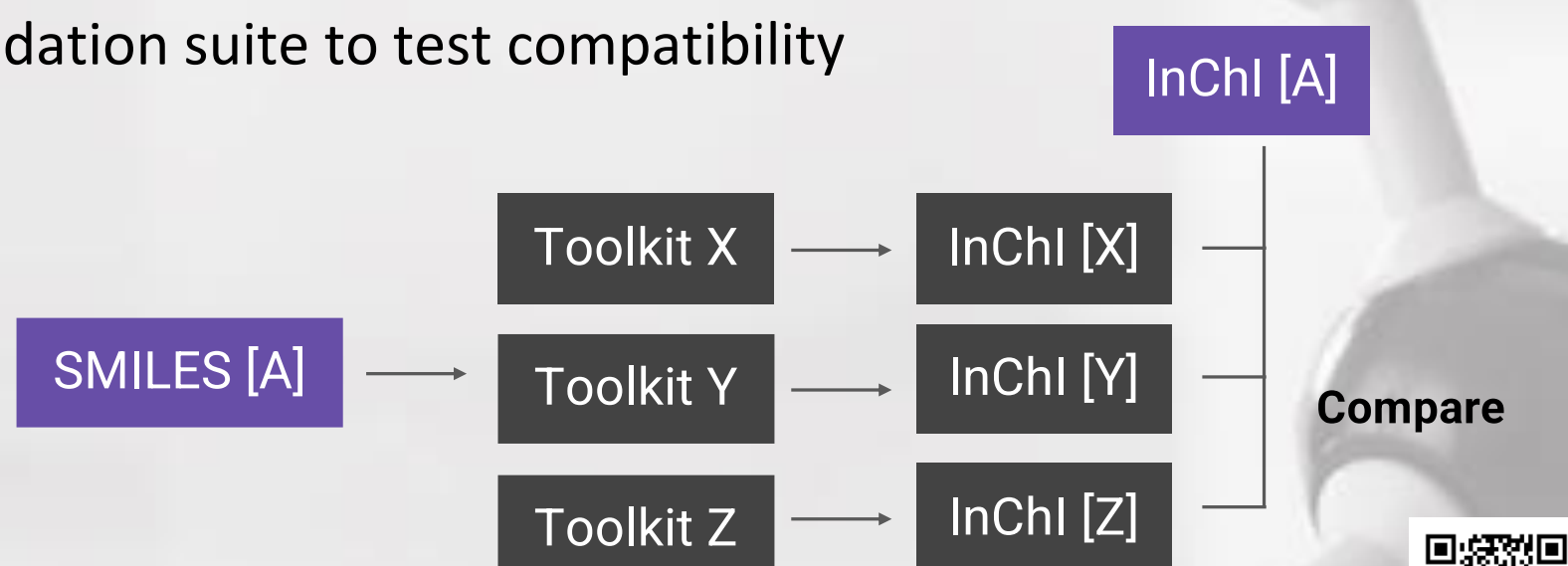
degruyter.com/journal/key/PAC/html



SMILES+

IUPAC project to develop formalized up-to-date open specification:

- Consistent **reading** of SMILES between toolkits
- Mechanism for community approved edits and extensions
- Validation suite to test compatibility



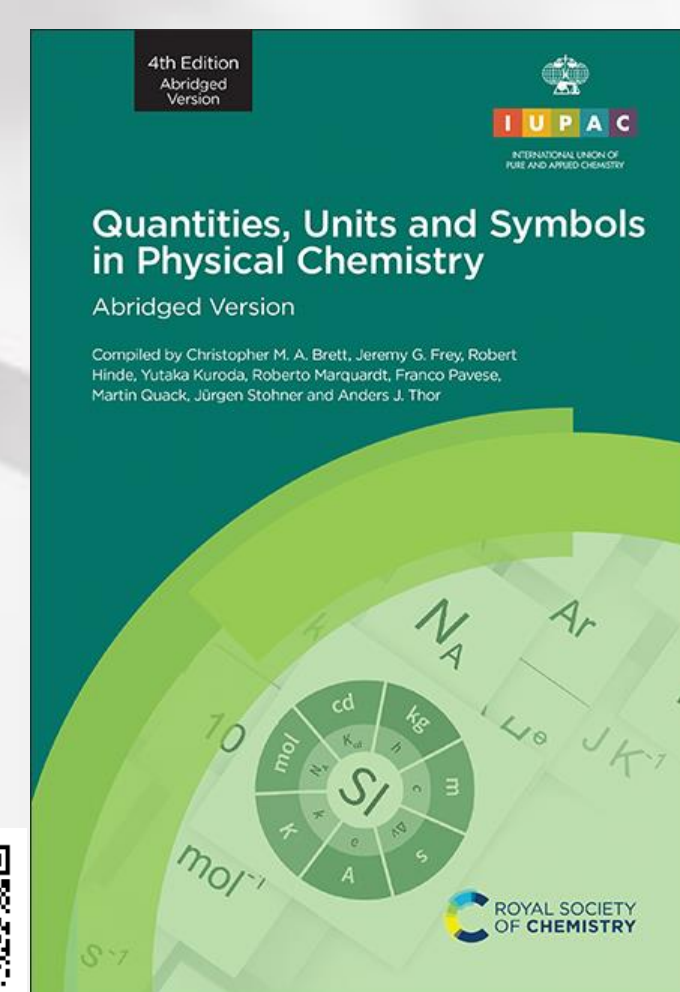
GitHub: https://github.com/IUPAC/IUPAC_SMILES_plus



Green Book

- Pending release!*
- New abridged edition covers the updated SI units and the most recent elements in the periodic table
- Suitable for students and teachers, scientists and organizations working across a multitude of disciplines

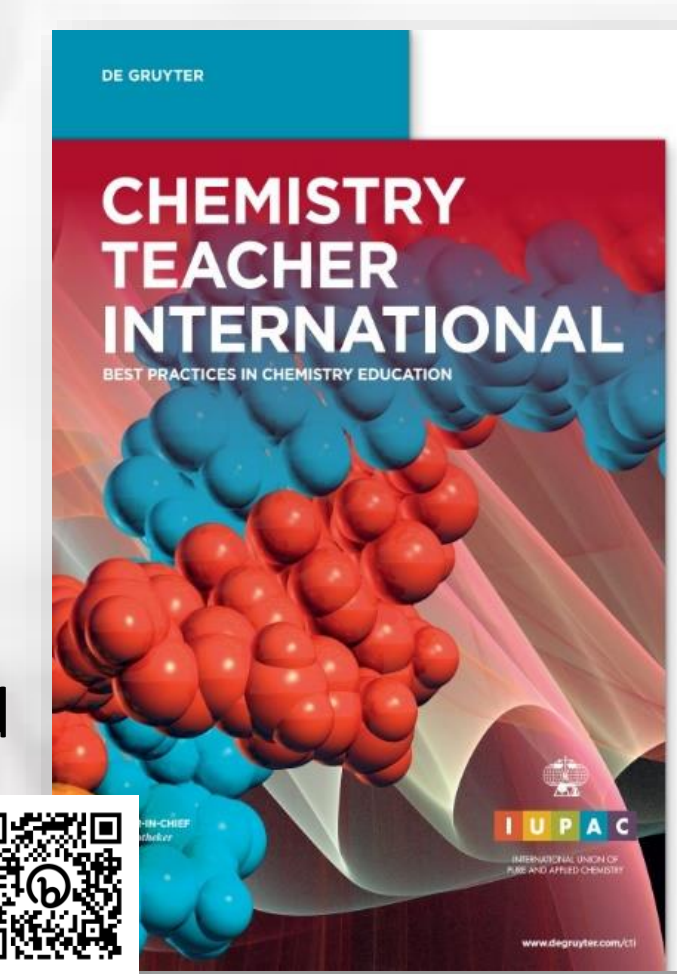
<https://books.rsc.org/books/edited-volume/286/Quantities-units-and-symbols-in-physical-chemistry>



Chemistry Teacher International

- Open access journal
- Est. by the IUPAC Committee on Chemical Education (2019)
- Objectives:
 - Bridging gap, research & education
 - IUPAC activities in education
 - International journal not linked to a specific area or nation

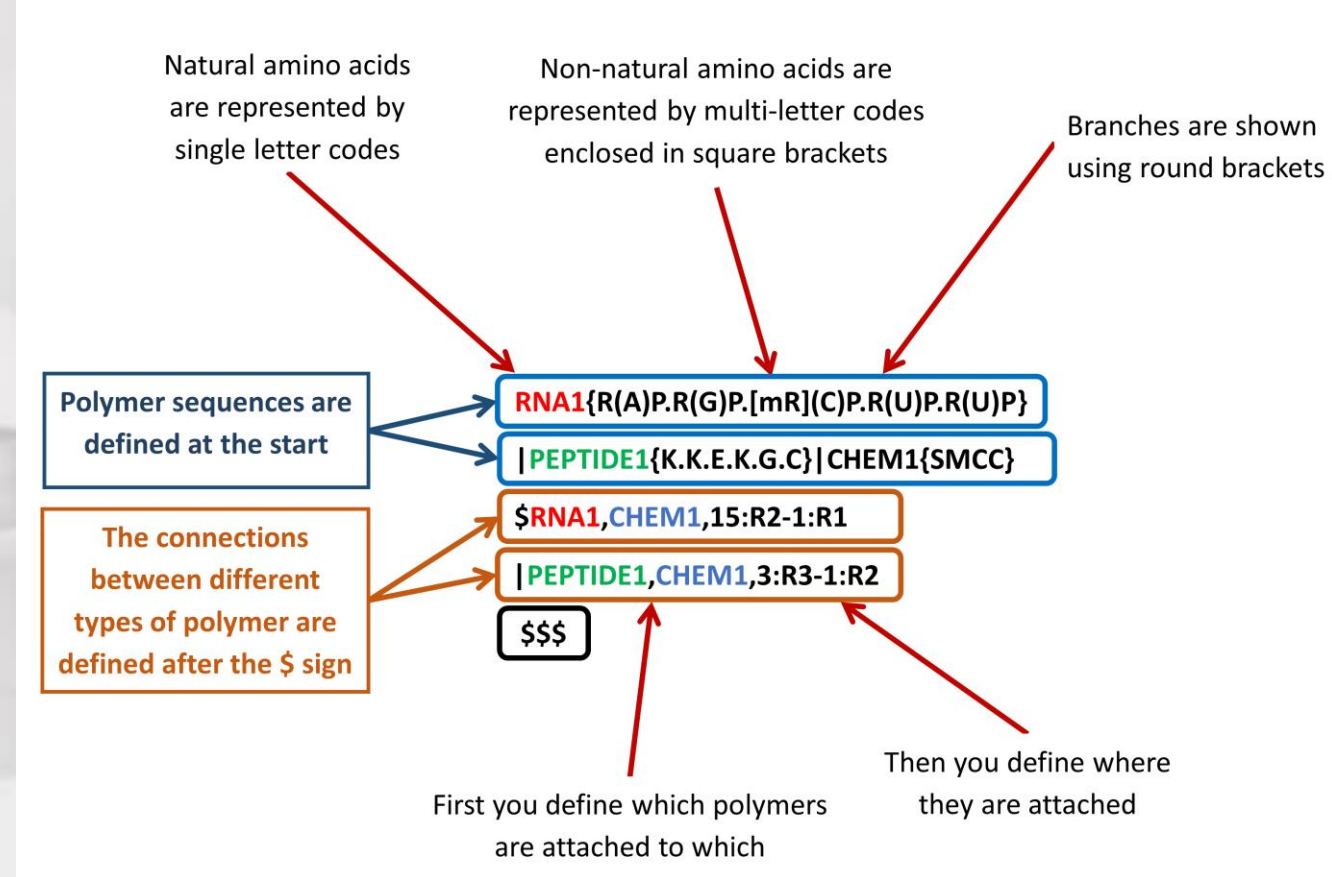
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HELM

Hierarchical Editing Language for Macromolecules

Pistoia Alliance



FAIRChemistry

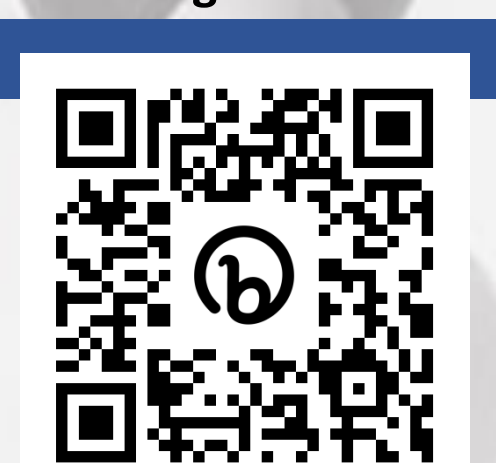
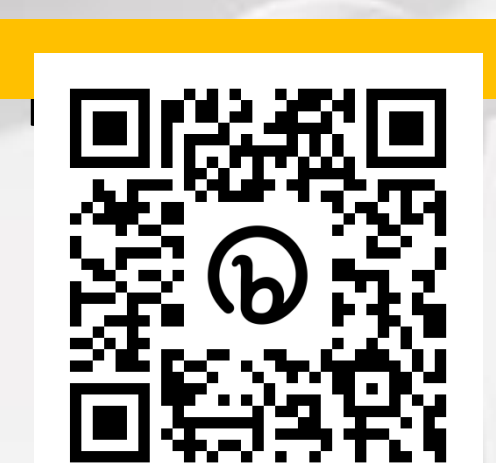
IUPAC standards support the FAIR data principles



D3.1 FAIR Chemistry Guidance

D3.2 FAIR Chemistry Training Cookbook

D3.3 FAIR Chemistry Protocol Services



bit.ly/IUPACDigitalRecommend

bit.ly/CookFAIR

bit.ly/ProtServices



Chemistry International

- Two-way exchange of information, news, and feature articles on IUPAC activities
- Free online to increase the visibility of IUPAC and our activities

<https://iupac.org/what-we-do/journals/chemistry-international/>



OTHER ONGOING ACTIVITIES

IUPAC Data Standards – FAIR updates

- Thermophysical & chemical properties
 - ThermoML XML format
 - Thermodynamics data reporting templates
- Spectroscopic data
 - JCAMP-DX ASCII legacy format
 - FAIRSpec: format-agnostic, FAIR minimal metadata standard
- Machine processable critically evaluated data compilations:
 - Isotopic Abundances and Atomic Weights
 - Solubility
- Digital representations:
 - Units of measure
 - Physical constants

Other publications activities

- IUPAC Standards Online*
 - Searchable database built from IUPAC's standards and recommendations, extracted from PAC
- Top 10 Technologies
 - showcase the value of Chemistry and to inform the general public as to how the chemical sciences contribute to the well-being of society and the sustainability of Planet Earth*
- Whitepaper on Blockchain technology in scientific publishing

FUTURE OUTLOOK

IUPAC Roadmap

Kickstart a Center of Excellence for Digital Chemistry Data Standards

Enable IUPAC

FAIRification plan for IUPAC standards; engage Divisions & collaborators

Sustain IUPAC

Blueprint for ongoing digital standards development & stewardship

Engage IUPAC

Color book on cheminformatics; chemical data curation workshop series, biennial conference on chemical representation

Partners & ACKNOWLEDGMENTS

