

IUPAC WorldFAIR Chemistry Managing Chemical Data Digitally



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Findable

Accessible

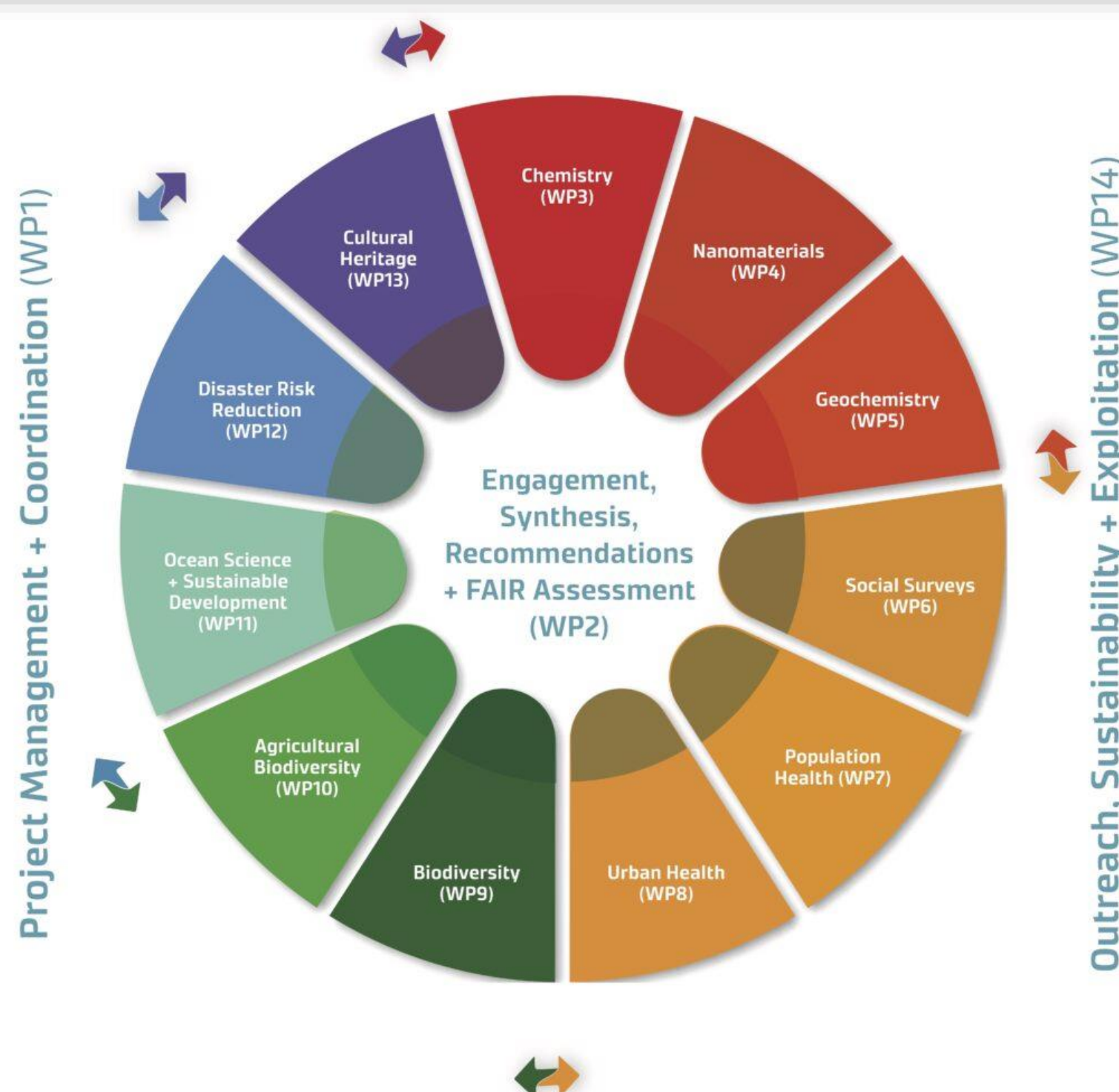
Interoperable

Reusable

WorldFAIR Initiative

Coordinated by CODATA and the Research Data Alliance, the WorldFAIR Initiative works with 11 case studies across disciplines to advance implementation of the FAIR data principles. The project seeks to develop a collective set of recommendations and a framework for FAIR assessment to improve Interoperability and Reusability of digital research objects. Particular emphases include:

- Adaptation and refinement of the **GO FAIR Implementation Profiles** methodology to assess alignment of FAIR enabling resources with broadly used technologies.
- Explore and establish parameters and practices for a **Cross-Domain Interoperability Framework** across the physical, social, agricultural and environmental sciences and the cultural heritage sector
- The case study for chemistry is led by IUPAC/ The Committee on Publications and Cheminformatics Data Standards (CPCDS) – see project 2022-012-1-024



IUPAC Roadmap

The goal of the WorldFAIR Chemistry project is to align IUPAC's chemistry data standards with the FAIR data principles through:

- Development of guidelines, tools and validation services that enable scientists to share and store data in a FAIR manner.
- Addressing gaps in standards that currently restrain chemistry in both academic and industrial areas, in particular taking advantage of developments in AI/ML.
- Engaging critical stakeholders in the adoption of standards and best practices to significantly increase the amount of chemical data available for all scientific disciplines.

Chair

• Leah McEwen

Members

• Evan Bolton

• Ian Bruno

• Stuart Chalk

• Simon Coles

• Jeremy Frey

• Wolfram Koch

• Fatima Mustafa

• Christopher

Steinbeck

• Antony Williams

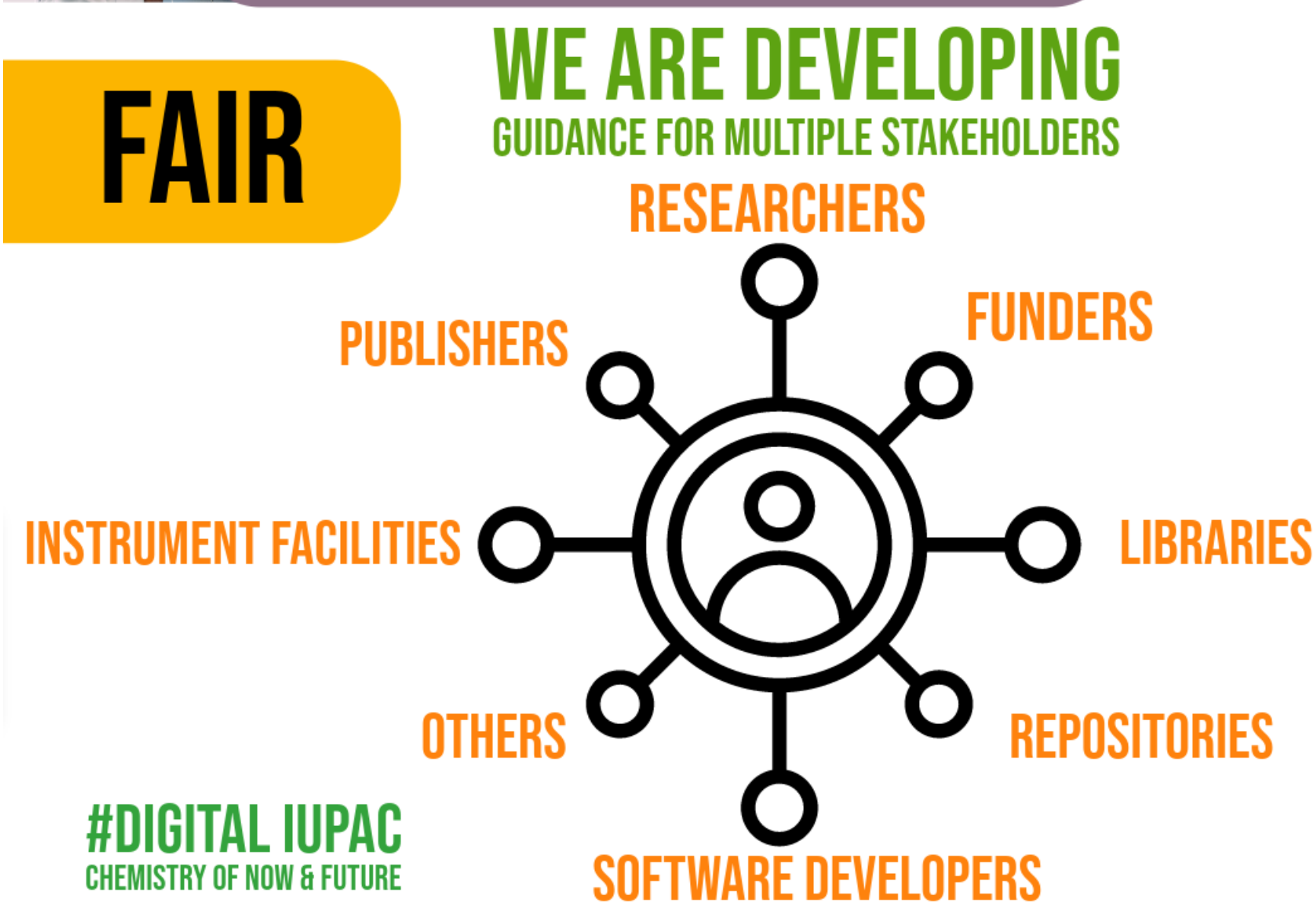
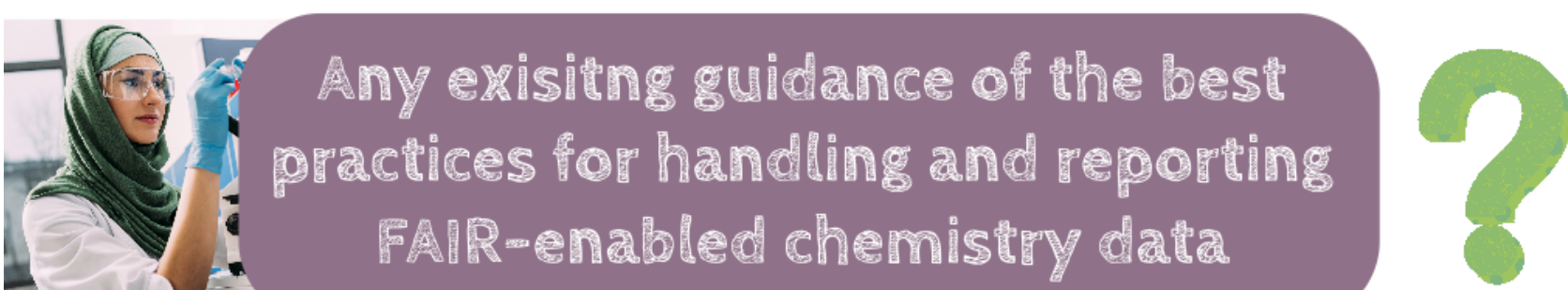
PROJECTS

Reporting Guidance Recommendations for FAIR chemical data reporting

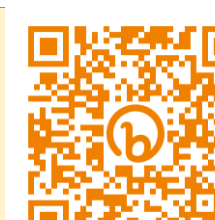
This project aims to:

- Develop guidance on best practices for handling and reporting FAIR-enabled chemistry data for different stakeholders.
- Bridge between general guidance for FAIR data and specific guidance for chemistry data types emerging through numerous activities in IUPAC standards projects and community-based use cases.

Reporting Guidance



Website



Report

Training Cookbook Digital recipes for managing chemical data

The FAIR Chemistry Cookbook is intended to:

- Support the broader community in understanding how to implement the FAIR data principles for chemical data.
- The site is designed to be a living resource through the addition of new content as strategies for implementing FAIR evolve and the sharing and reuse of FAIR chemical data continues to increase.



Website



Demo



Feedback

Protocol Services Standardized programmatic access to chemical information

These protocols based on IUPAC standards aim to support web services that:

- Confirm chemical identity.
- Assess machine-readability of chemical data and metadata representation of chemical moieties.
- Query registered resources with different scopes and capabilities.

Structure Validator

Is the chemical structure OK?



Website



Demo



Feedback

Outreach Activities

- ❖ Webinars series
"What is a chemical?", Fall 2022
ChemVoices, May 31, 2023
- ❖ Conference sessions
Research Data Alliance
(March 2023, October 2023)
SciDataCon, October 2023
International Data Week 2023
ACS Fall 2023
- ❖ Workshops
ACS Spring 2023
Pistoia Alliance 2023
- ❖ Presentations
FAIR Convergence Symposium,
October 2022
Australian Vocabulary Symposium,
November 2022

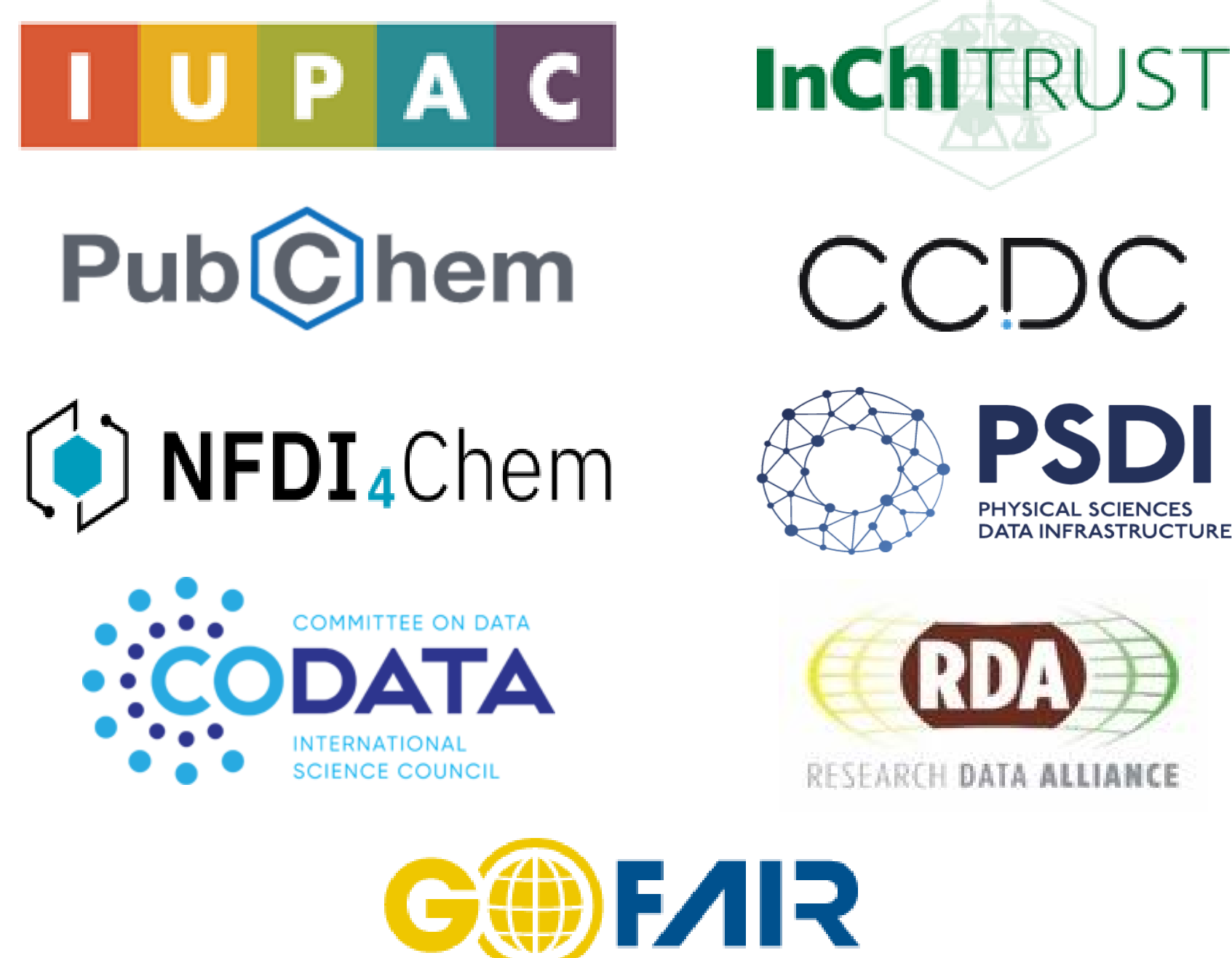


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