

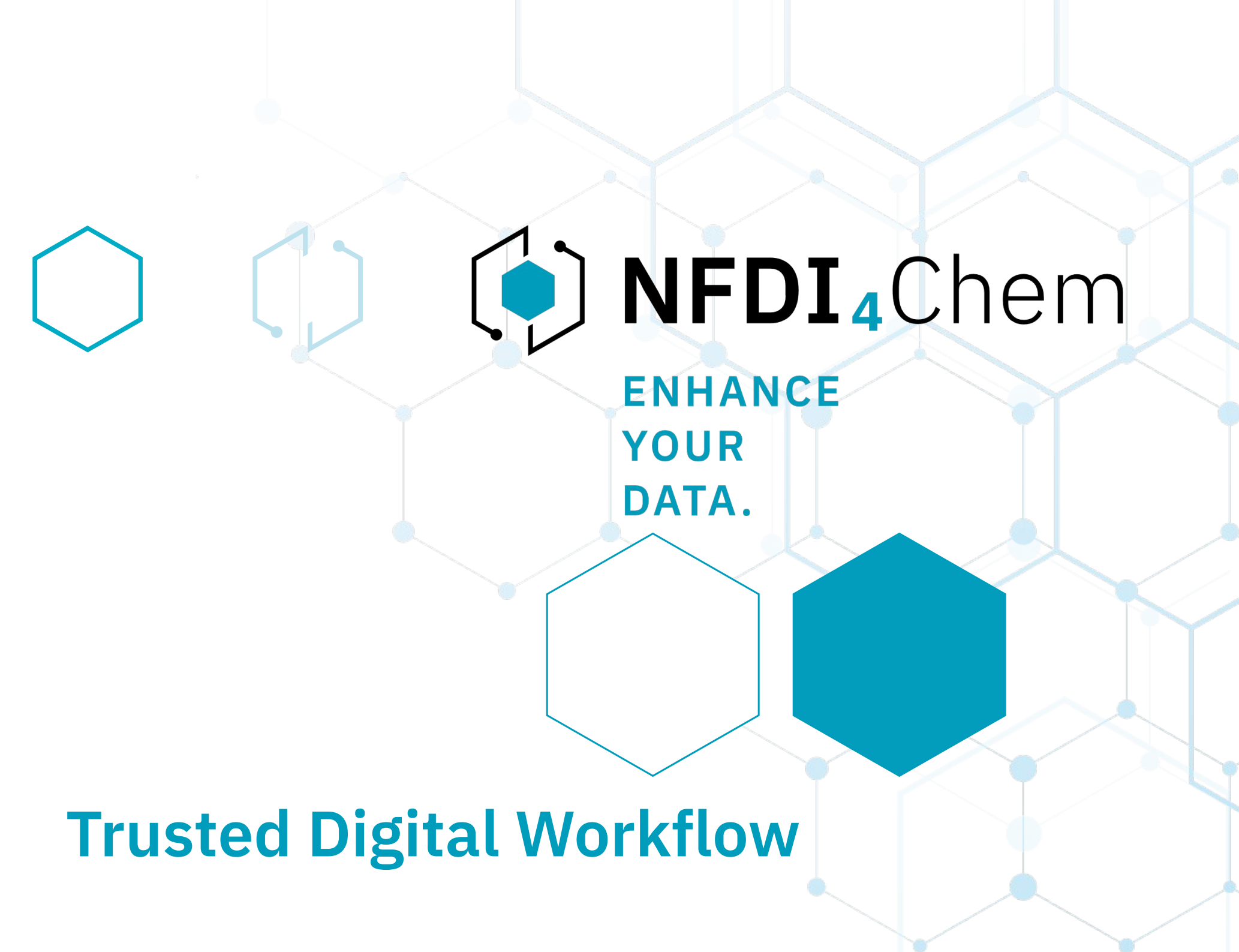
Trusted Chemistry Data for the Digital Age: Inside NFDI4Chem's Federated Infrastructure

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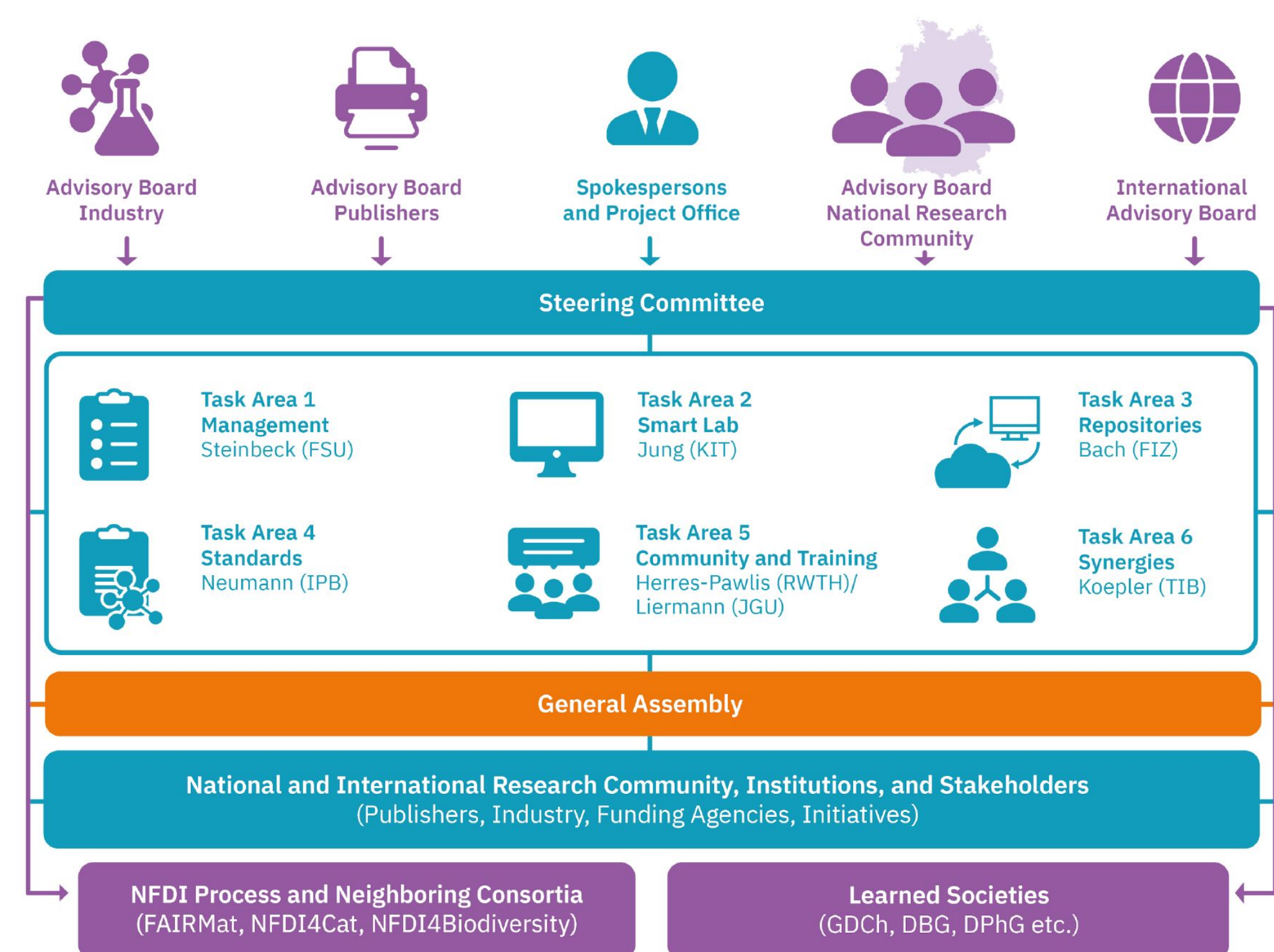
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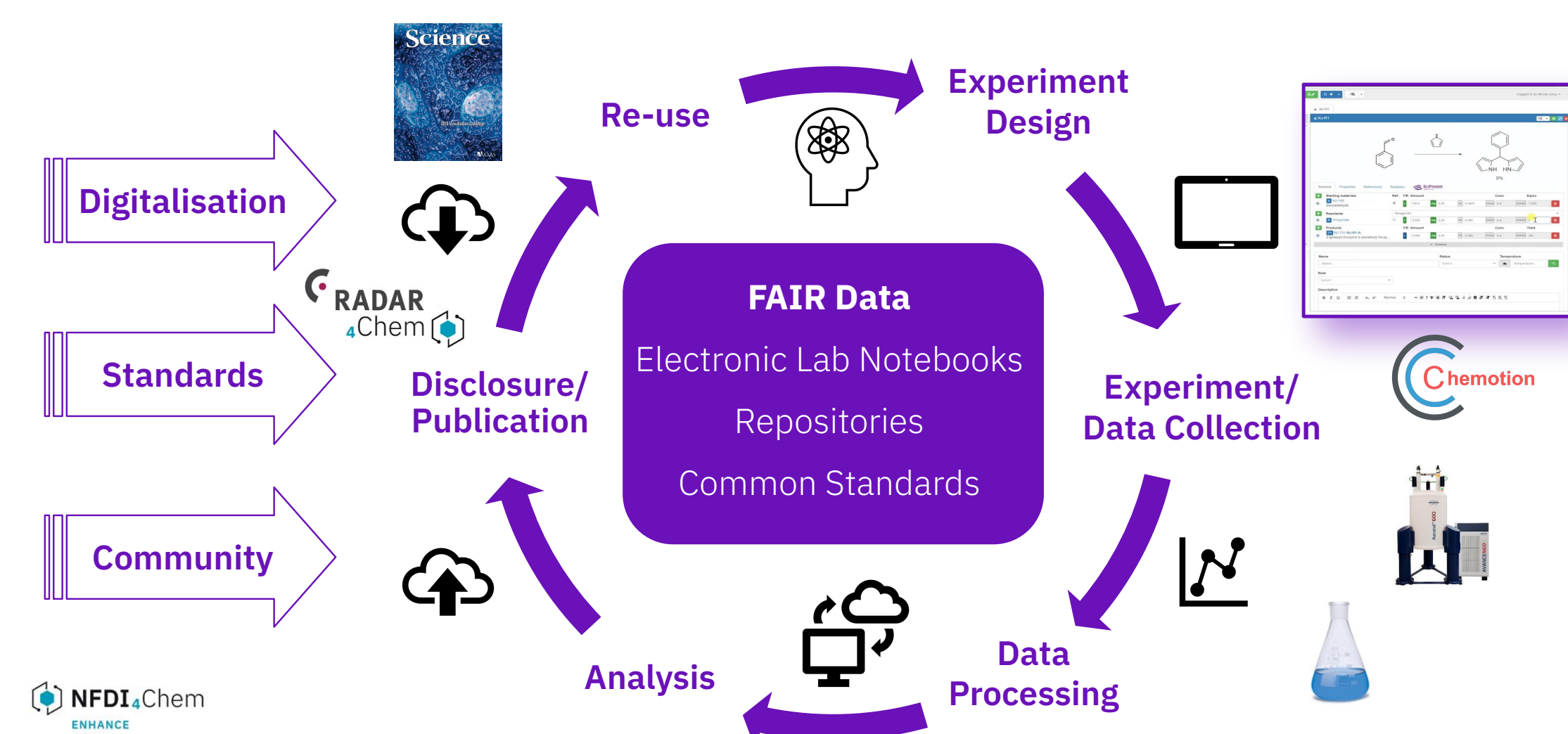
NFDI4Chem Governance Structure



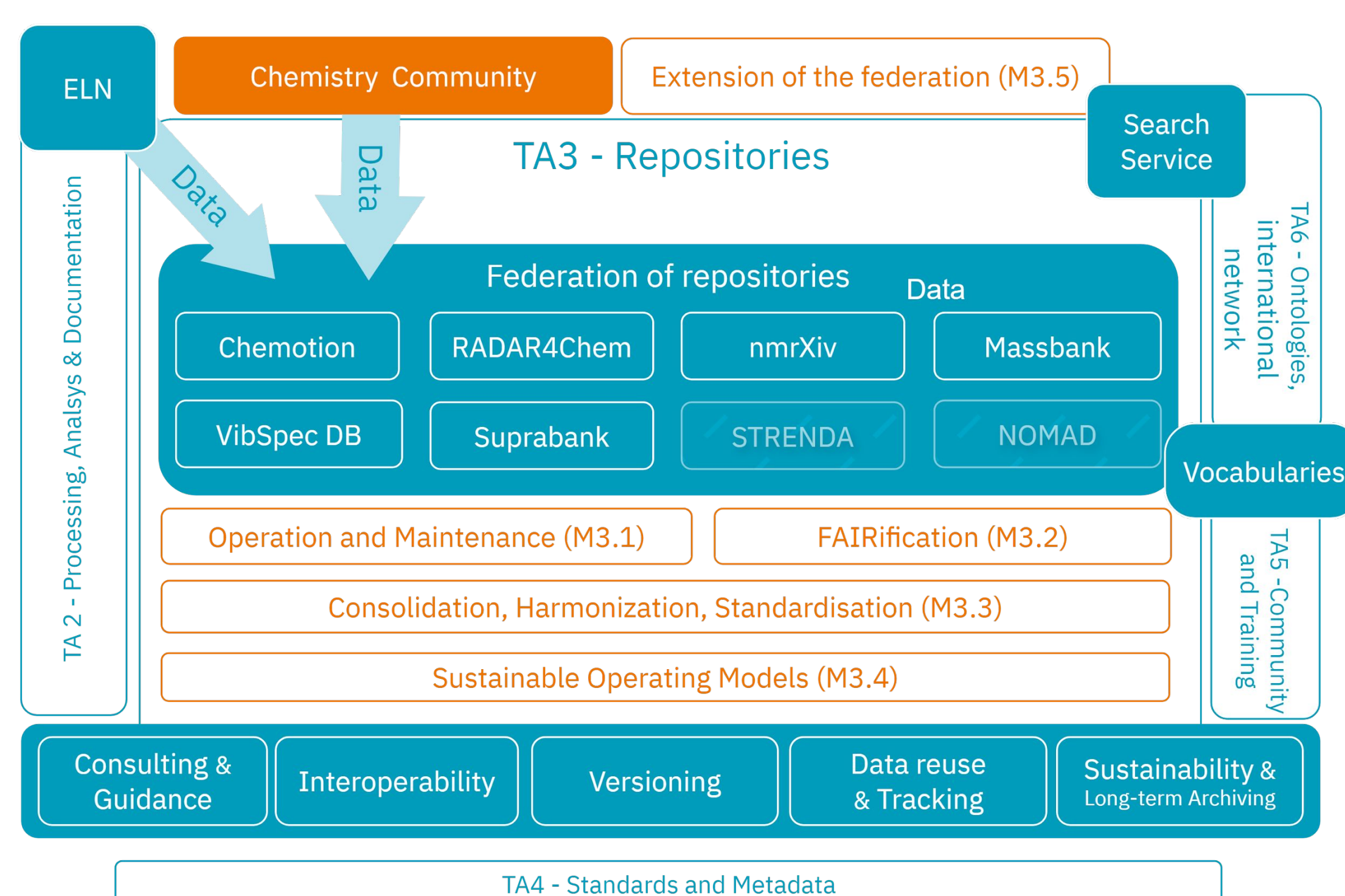
NFDI4Chem's Vision

- Strengthening the research data ecosystem
- Leading the development of MI standards and machine-readable metadata
- Advancing Smart Laboratory Environments
- Driving cultural and digital transformation in the chemistry community
- Creating interdisciplinary synergies
- Enabling data reuse and AI in chemistry

Trusted Digital Workflow



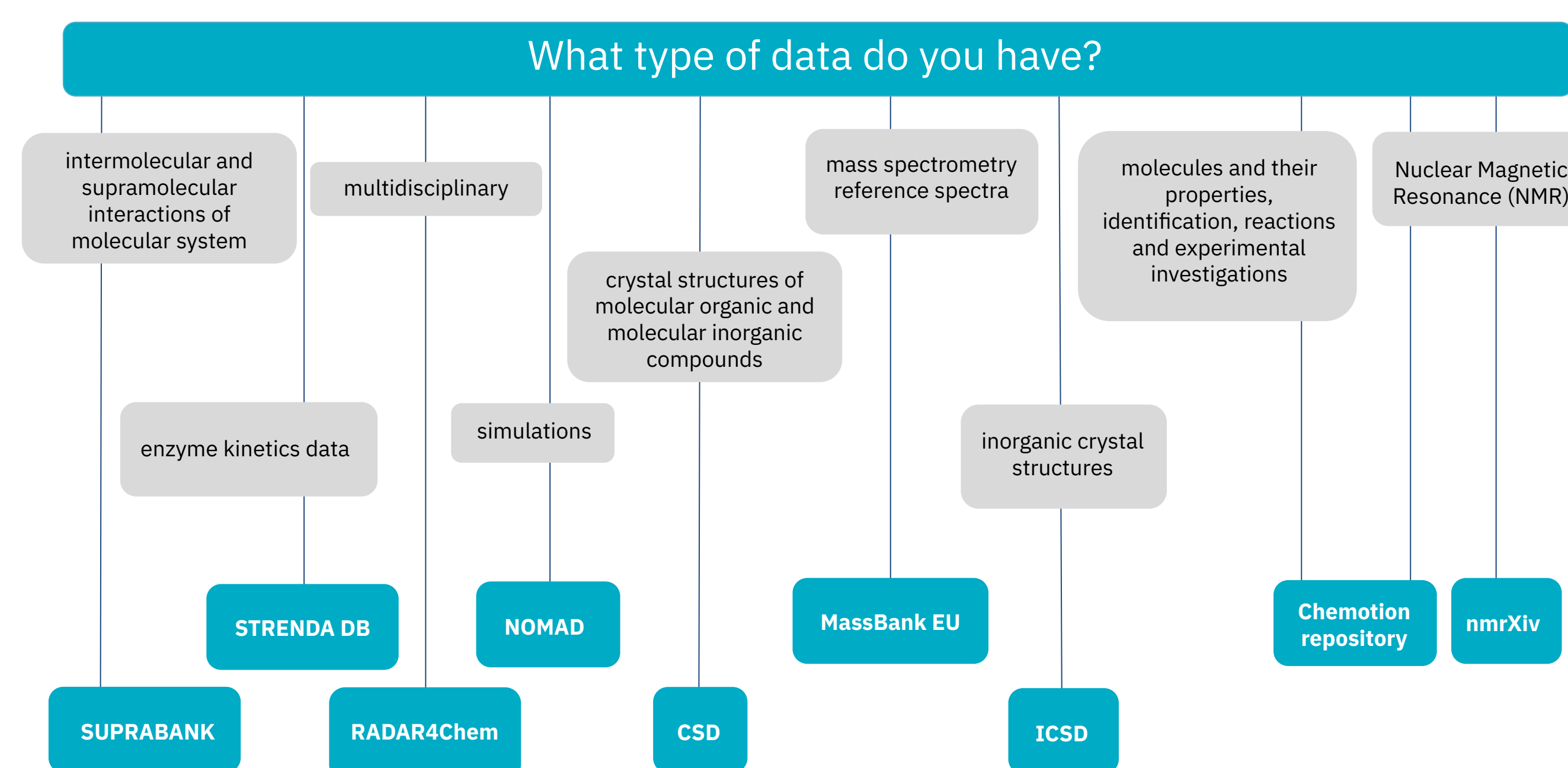
Task Area 3 (Repositories)



Federated Repositories

- Cover all relevant Data Types in Chemistry
- Semantically rich contextual metadata
- Discovery, Access & Reuse
- Secure Data Deposition
- Long-Term Archiving
- Effortless Data Publishing
- Interoperability by Design
- Reliable, trusted Services
- Seamless Smart-Lab Integration

How to choose the right Repository



Common Features Across All Repositories

Metadata & Interoperability

- Providing DOI registration via DataCite
- Implementing our *Minimal Information on Chemical Investigations* (MICHl)
- Supporting metadata in modern structured formats (e.g. JSON-LD, Schema.org)
- Offering embargo options or controlled pre-publication access (e.g. for reviewers)
- Enabling interoperability with external tools (e.g., Chemotion ELN, instruments, or domain tools)
- Supporting metadata harvesting mechanisms (i.e. via OAI-PMH) allowing seamless integration in aggregators and our NFDI4Chem search

Authentication & Access

- Supporting Single Sign-On (SSO) authentication (DFN-AAI, Shibboleth, OpenID Connect, ORCID, GitHub, etc.)

FAIRness & Findability

- Providing search capabilities and/or advanced discovery (e.g., structure search, knowledge graph, vocabularies)

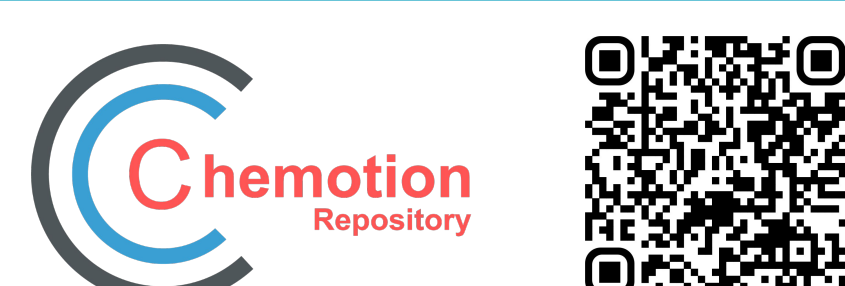
Community/Domain Orientation

- Recommended by scientific journals (Angewandte Chemie, Wiley journals, Journal of Natural Products etc.)
- Supporting or integrating with controlled vocabularies / domain standards



- Launched in 2022
- Guaranteed **>25 years** retention period
- Enhanced **F-UJI Scores** up to 87%
- Data **upload** via browser or WebDav clients
- RADAR **knowledge graph** and support of RADAR **SPARQL** endpoint
- Chemotion ELN -> RADAR4Chem seamless **data transfer** and **publication**
- **Large volume** data: resumable data downloads after interruptions
- **Metadata enhancement**: RADAR Keywords Services (TS4NFDI)
- **FAIRness** assessment: FAIRway Service (**AI**)
- Available for EU countries, Switzerland and UK
- 40 **Workspaces** and 17 **Institutions**
- 166 **Datasets** (each of it contains **several data**)

Partner, Unterstützer, usw.
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NFDI4Chem is supported by DFG
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- Launched in 2014
- **Data transfer** and publication from Chemotion ELN possible
- Data Federation **Tracker software** to record and monitor data transfer processes
- High-quality data ensured through **curation workflow**
- **Streamlined collaboration**: assign group leads, auto-add to submissions, adjust affiliations, and standardise with Global & Review Labels
- **Domain Specific** metadata
- **One-Click** Metadata and Data **Downloads**: Export human-readable Excel files, as well as JSON-LD and RDF formats for data exchange.
- **Repository search** and **structure search** functions
- **Analytics** enabled via Matomo
3101 **samples** (2022) → + **2288** (2025)
1362 **reactions** (2022) → + **1766** (2025)
10888 **analyses** (2022) → + **12661** (2025)



- Launched in 2023
- Open-source NMR spectra processing tool - **NMRium integration**
- Ready-to-use **NMR data management platform** to host your raw instrument data and processed files for free and provides you with tools and services to analyse data
- **Community-trusted** repository for NMR data deposition
- **Publication friendly** with spectra level DOIs, embargo mode and reviewer's access links
- **Analytics** enabled via Matomo
- Evolving support of domain Minimum Information Standards (**MICHl** Standard for Reporting Liquid-State NMR Experiments of Small Molecules - **MARGARITAS**)
- Leveraging **Controlled Vocabularies**
133 **projects** (2025)
1095 **compounds** (2025)
5497 **spectra** (2025)