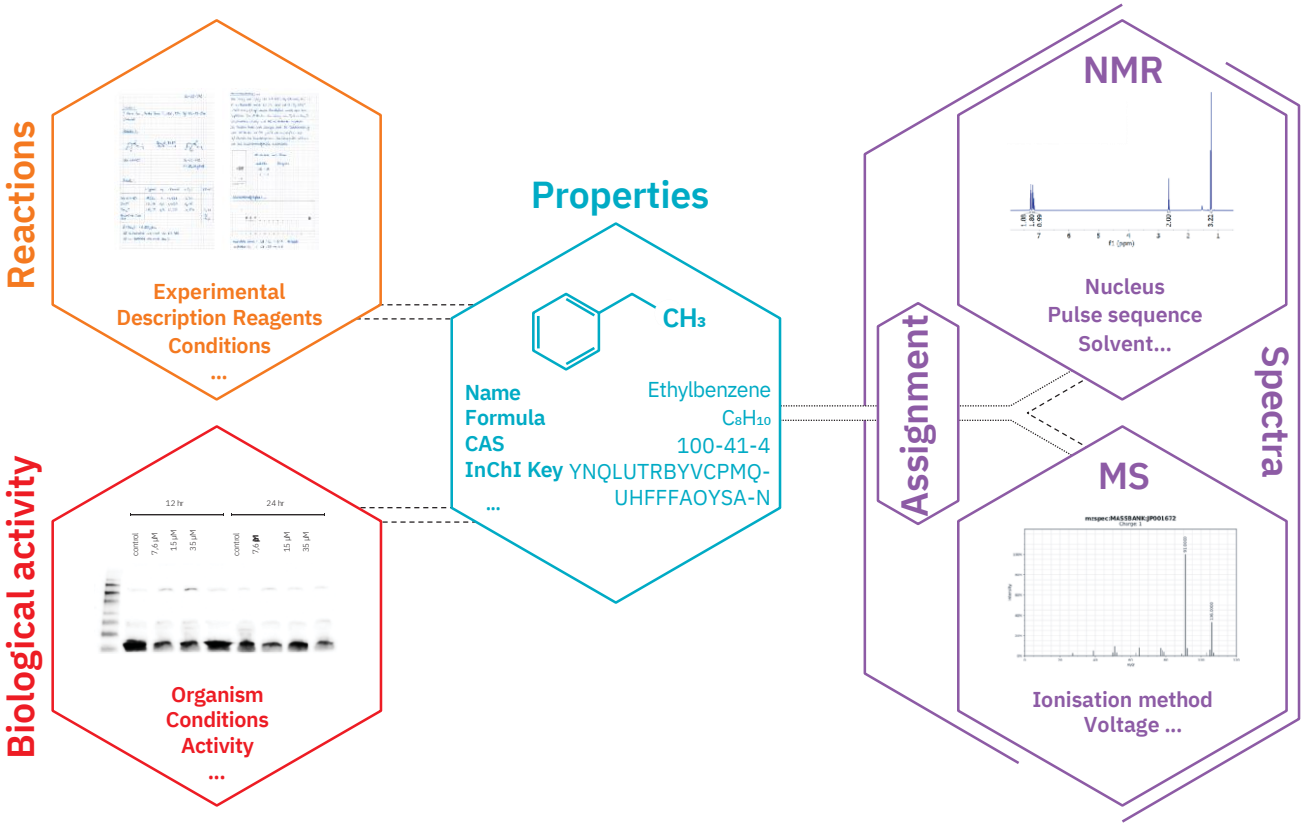
NFDI4Chem

ENHANCE
YOUR
DATA.

NFDI4Chem: vom chemischen Forschungsdatenmanagement zur digitalen Chemie

S. Herres-Pawlis, F. Bach, N. Jung, O. Koepler, J. Liermann, S. Neumann, M. Razum, C. Steinbeck

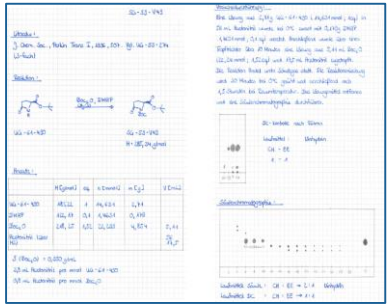
Molecules and related meta(data)

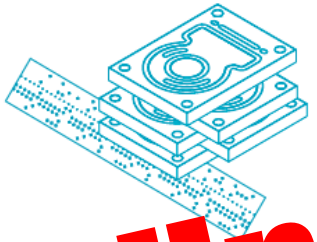


Status Quo

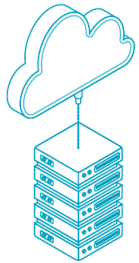
Findable
Accessible
Interoperable
Reusable

Analogue / Digital

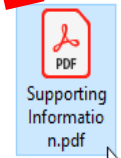


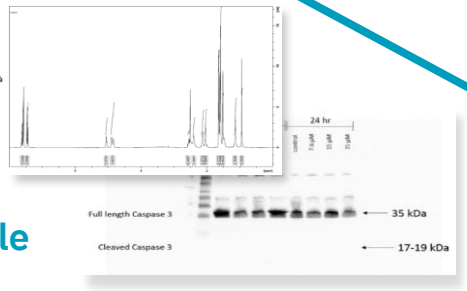


Digital



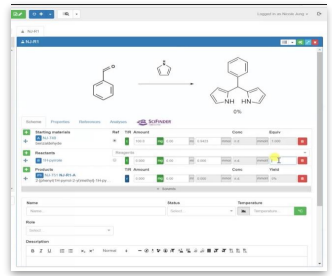
UnFAIR





Not machine readable

Our Vision



Digitisation

Standards

Community

Re-use

Experiment Design

Experiment/ Data Collection

Data Processing

Analysis

Disclosure/ Publication

FAIR Data

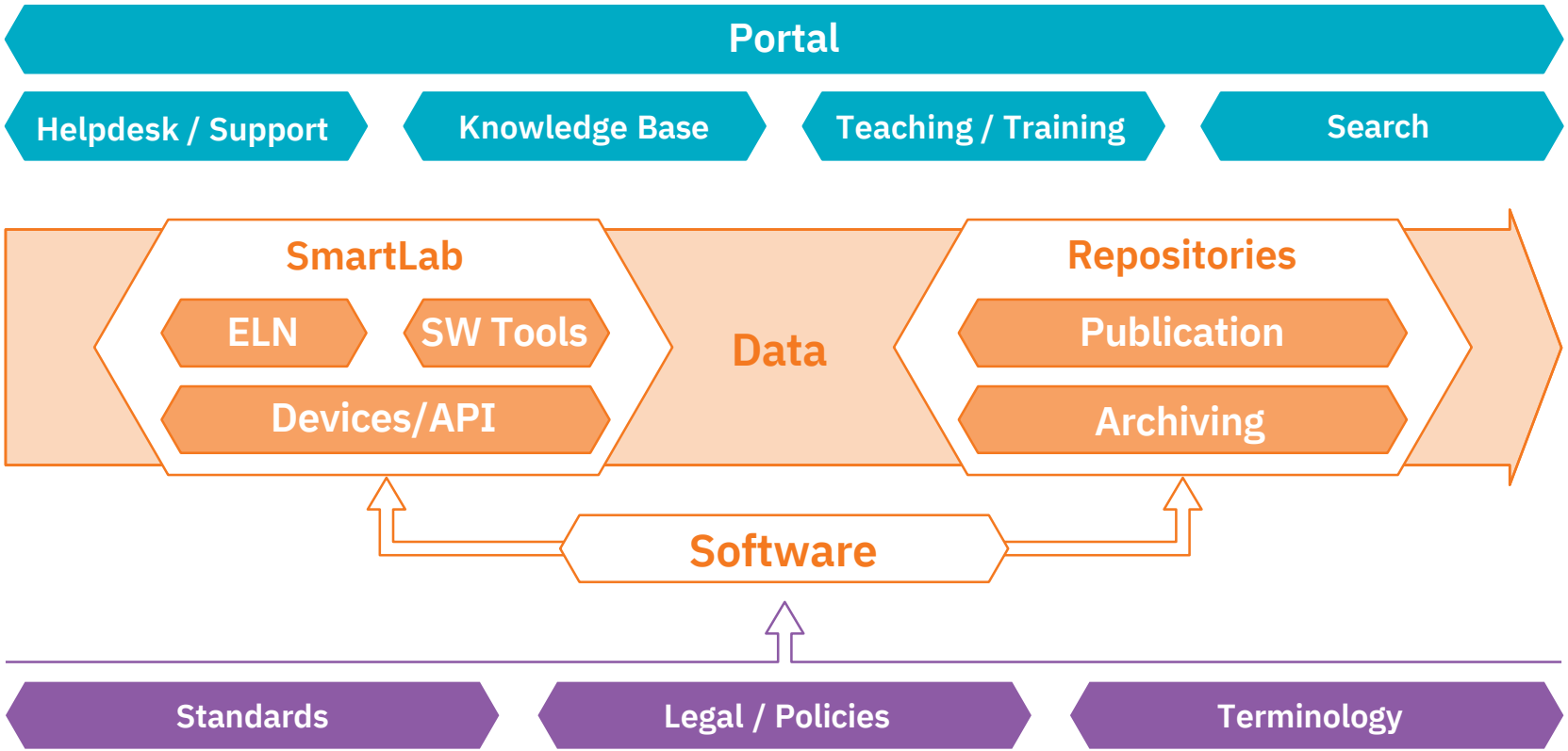
Electronic Lab Notebooks

Repositories

Common Standards

What is our Strategy?

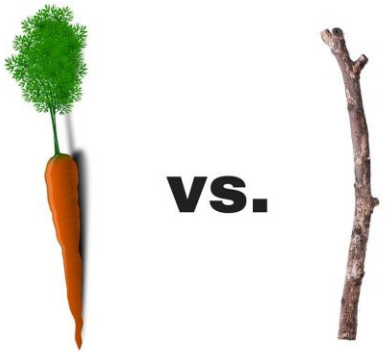
Strategy


Portal
Helpdesk / Support
Knowledge Base
Teaching / Training
Search
SmartLab
ELN
SW Tools
Devices/API
Data
Repositories
Publication
Archiving
Software
Standards
Legal / Policies
Terminology

Working with publishers and funding bodies

- Close collaboration with IUPAC on publications and chemoinformatics data standards
- CRDIG Chemistry Research Data Interest Group, Research Data Alliance (RDA)
- Chemistry GO FAIR Implementation Network ChIN (IUPAC, CRDIG)
- Editors4Chem – working with publishers to set FAIR requirements for publications
- Working with funding bodies to determine FAIR requirements to fund research

DFG Deutsche Forschungsgemeinschaft



Working with IUPAC and the InChI Trust

- Close collaboration with IUPAC on publications and chemoinformatics data standards
- Close collaboration with the InChI Trust

- Problem of the International Chemical Identifier (InChI), version 1.06: disconnection of metal bonds leads to errors in databases and low acceptance of ELNs in inorganic chemistry
- Integration of molecular inorganic chemistry into the next InChI version by the non-disconnection approach (two programmers in Aachen), beta-version available in winter 23/24
- New webdemo already online:
  https://iupac-inchi.github.io/InChI-Web-Demo/

VolkswagenStiftung

Editors4Chem

- Forum for journal editors and RDM experts to set publication standards in an RDM context
- First Editors4Chem workshop November 2021: **18** Editors in chief from **5** publishers representing **25** Journals
- Next Workshop:
  - **2nd November 2023**

EDITORS 4Chem

Are you an editor and interested in joining?

Contact us at helpdesk@nfdi4chem.de

Why is there a reluctance to publish data?

- Close collaboration with IUPAC on publications and chemoinformatics data standards
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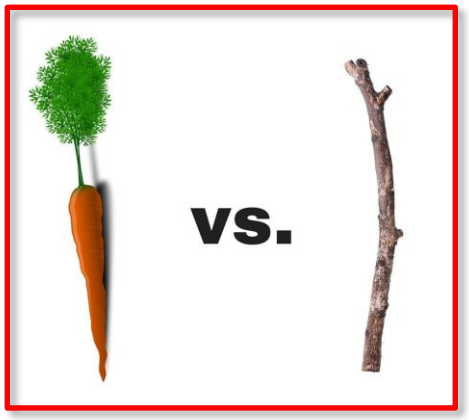
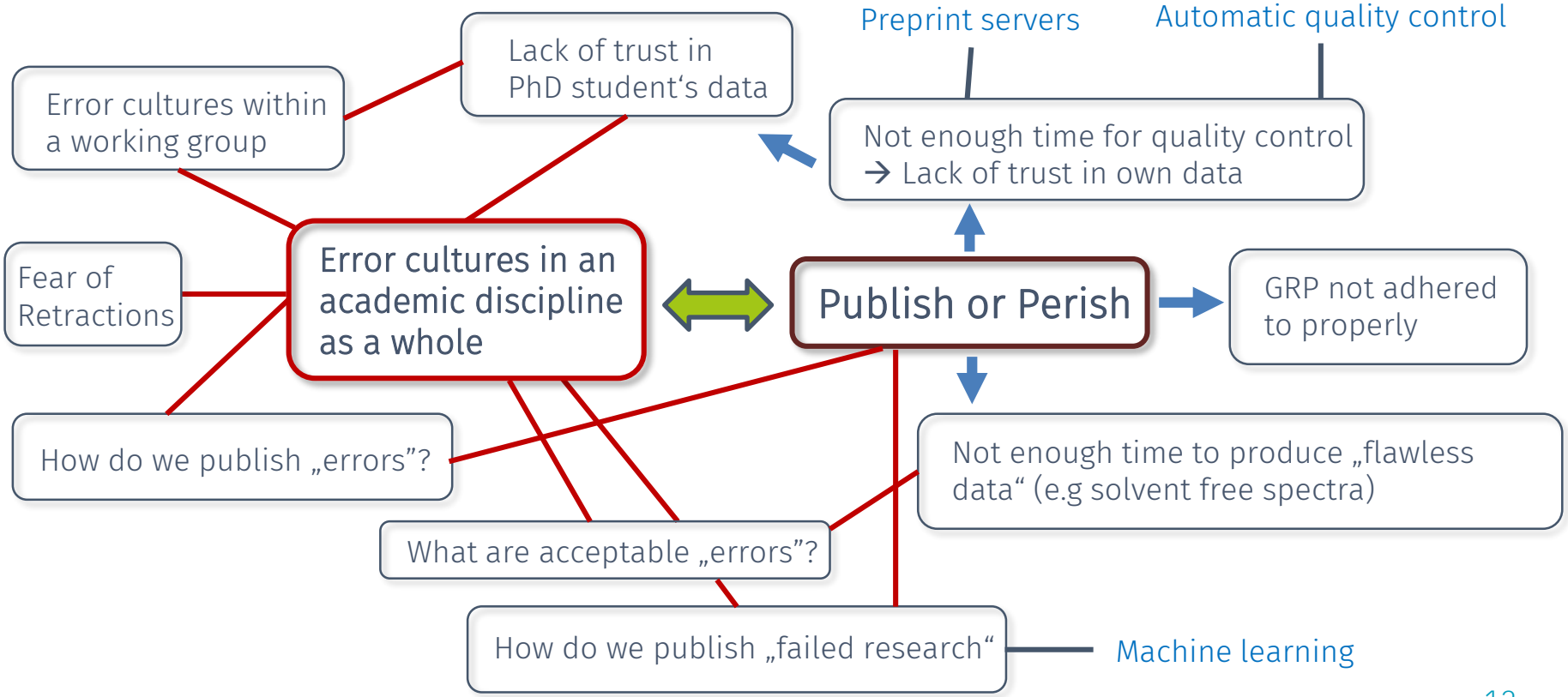


Why is there are reluctance to publish data?

„I am afraid of publishing my data because others may discover mistakes in my data or research which in turn could detrimentally impact my career“

Cultural Change, Publish or Perish, Error Cultures

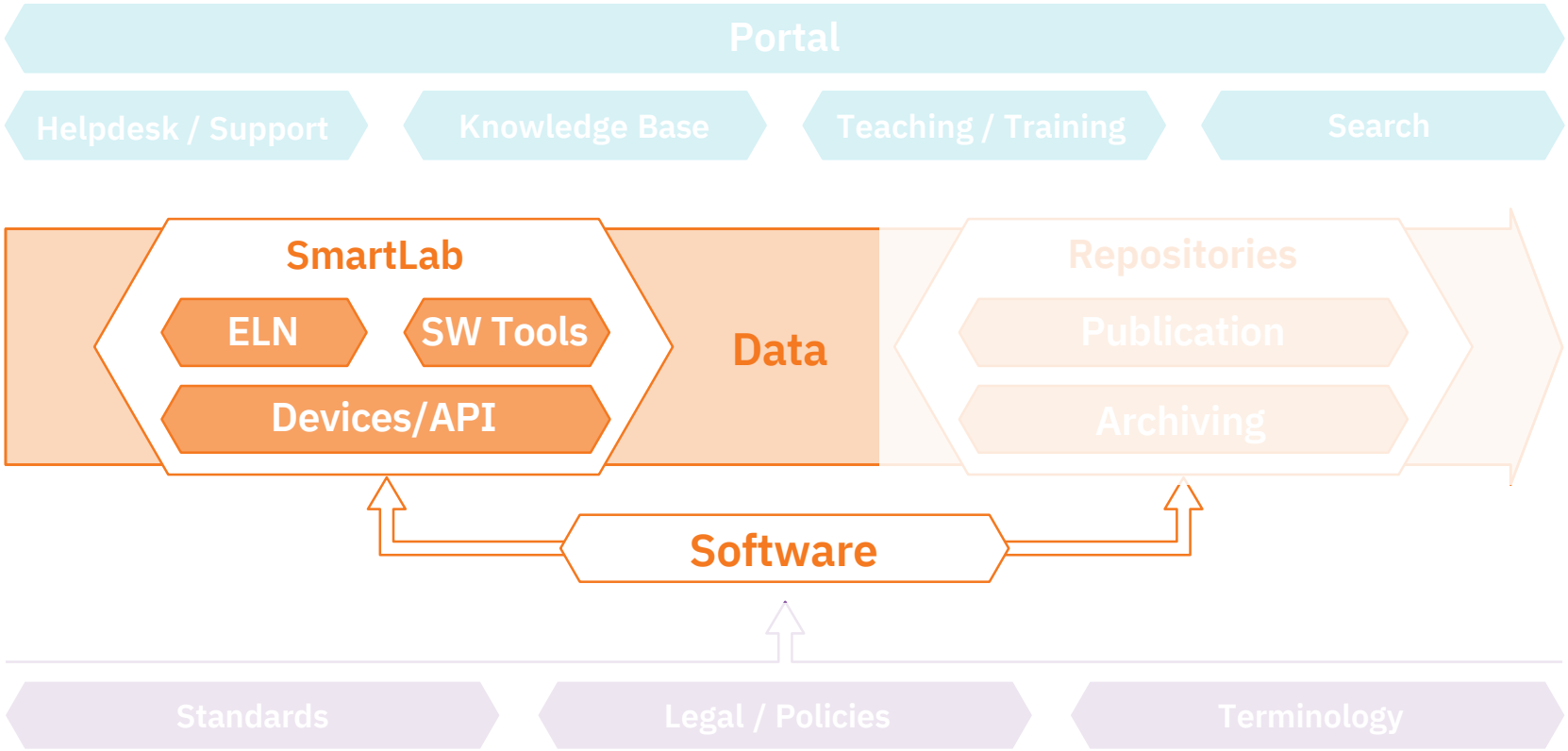


What can the NFDI realistically achieve?

- Systemic issues deeply rooted into academic culture → change won't happen over night
- NFDI working group on error cultures has identified two key areas, where we can make a realistic contribution.
  - **Awareness:** Raise awareness in events, social media for these issues – the more people talk openly about these issues, the more likely actual change can happen
  - **Error cultures in academic working groups:** Analysis and summary of concepts regarding error cultures from a non-academic background and how these might transfer to academia. A whitepaper is currently being written by NFDI members from sociology and psychology backgrounds.

What do we offer?

ELNs & Repositories

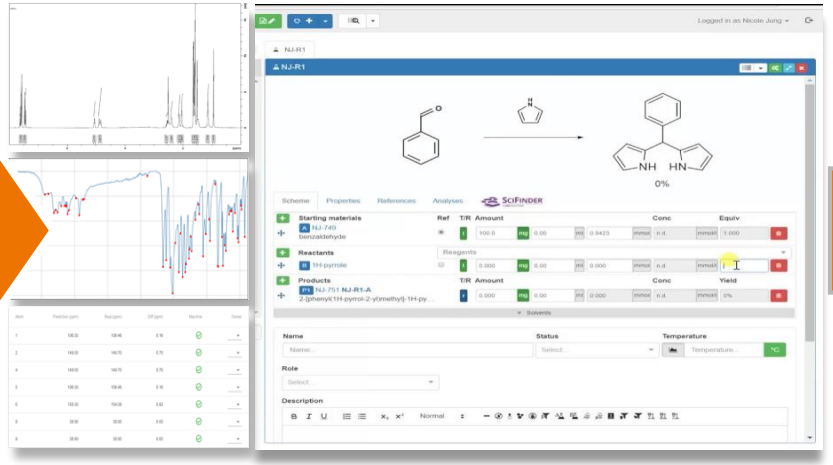


Smart Lab - Seamless Data Flows

Devices

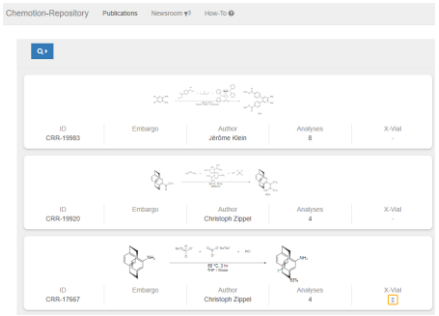
Data

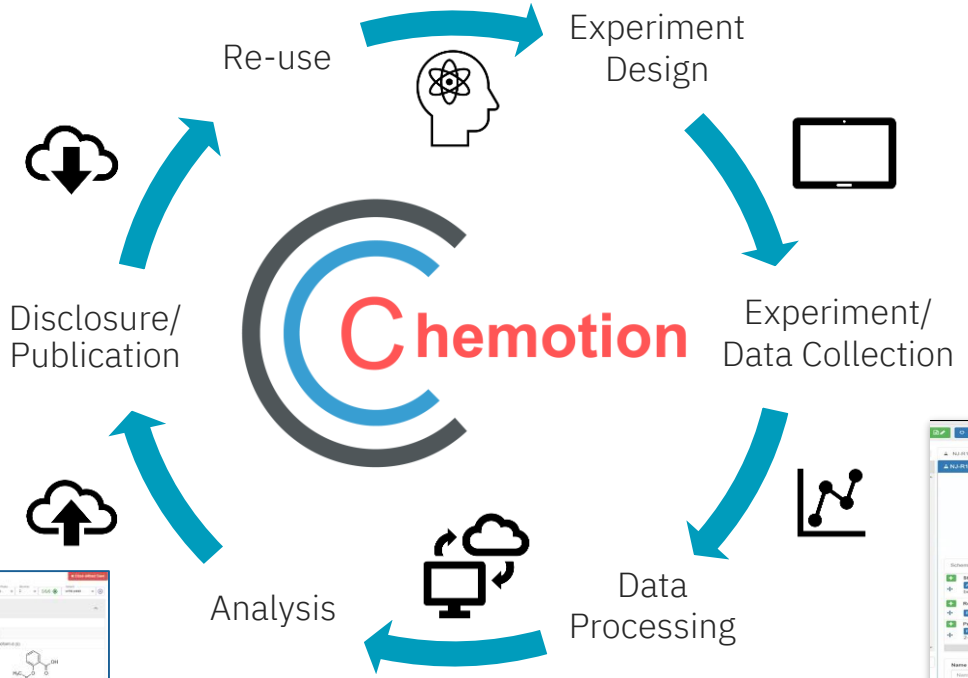
Electronic Lab Notebook (ELN)

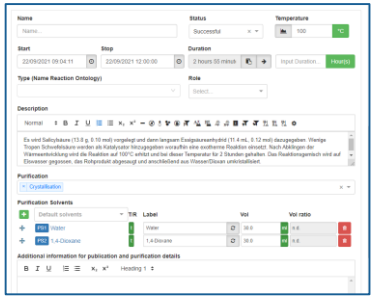


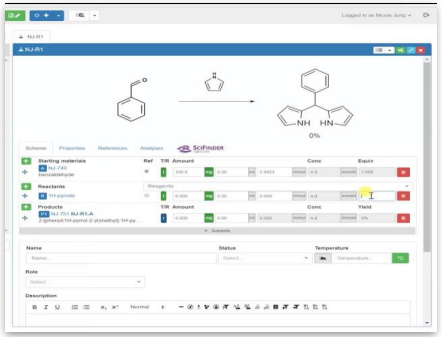
Federated Repositories

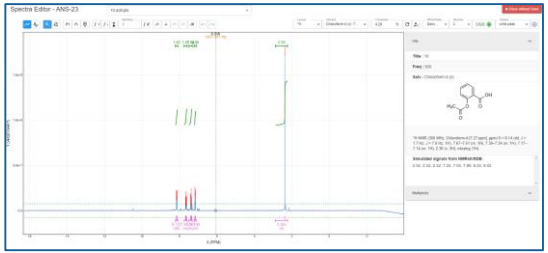
Chemotion – ELN & Repository











Chemotion – Quick Facts

- Developed by Karlsruhe Institute for Technology in collaboration with NFDI4Chem partners
- ELN for Chemistry (and related disciplines)
- Main Focus: Realisation of the FAIR data principles
- Advantages:
  - Open-source → Free!
  - Browser-based (Chrome)
  - Drawing of chemical structures
  - Creation, description and documentation of reactions
  - Analysis of spectra & characterisation of samples
  - **Automatic implementation of FAIR data principles (e.g. open formats, structured metadata)**

Chemotion

https://www.chemotion.net/

Chemotion - Setup

Back-up Servers

If possible, involvement of departmental IT-services.

Ingestion of data

Conversion to open formats

Control via VNC client

Back-up

Chemotion ELN

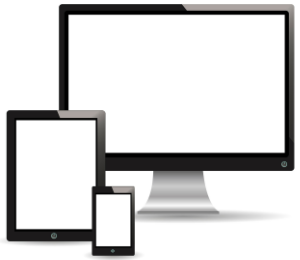
Virtual Machine

/ Server

Devices

Planning, documenting

Data analysis



Users (browser access)

RADAR 4Chem

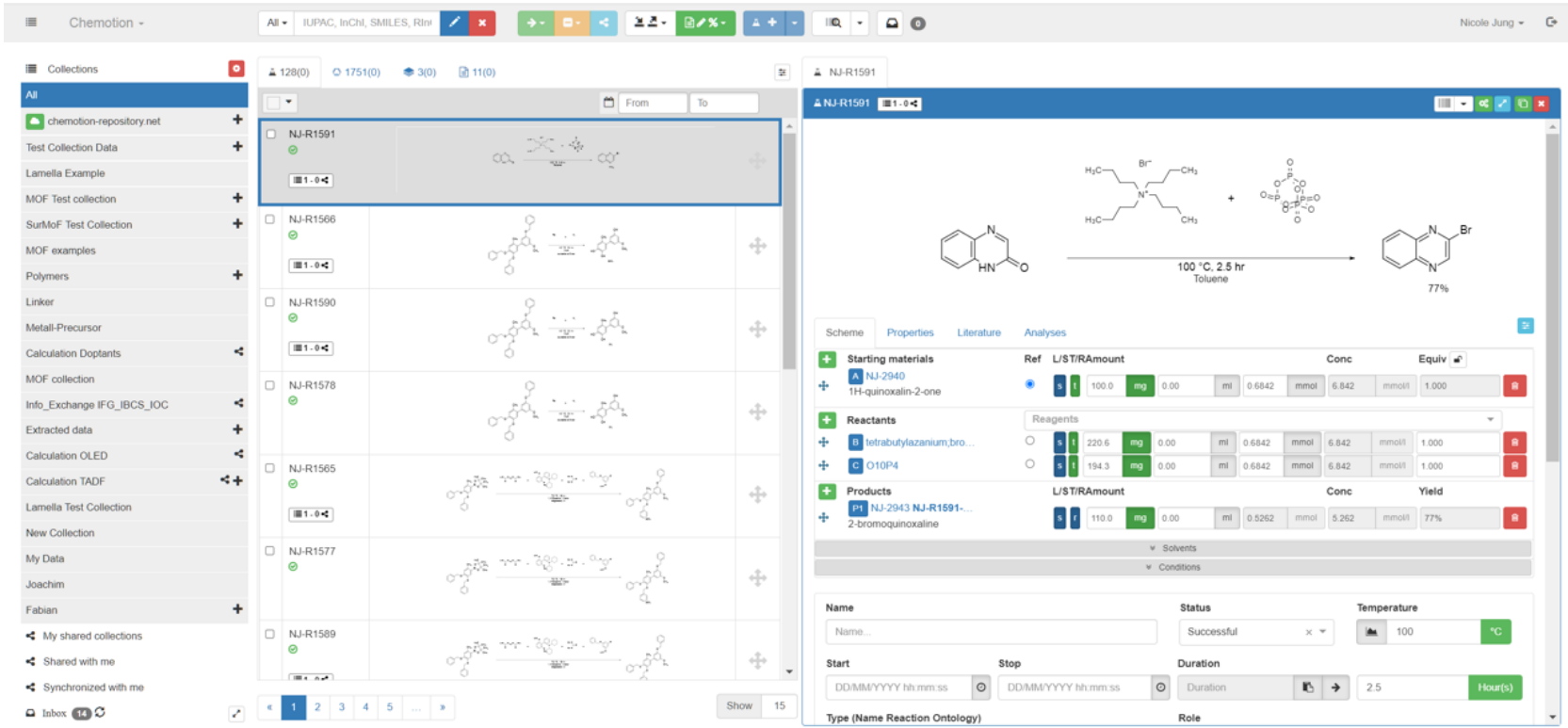
Chemotion Repository

Repositories

Data publication:

Publication collections or individual datasets in open repository

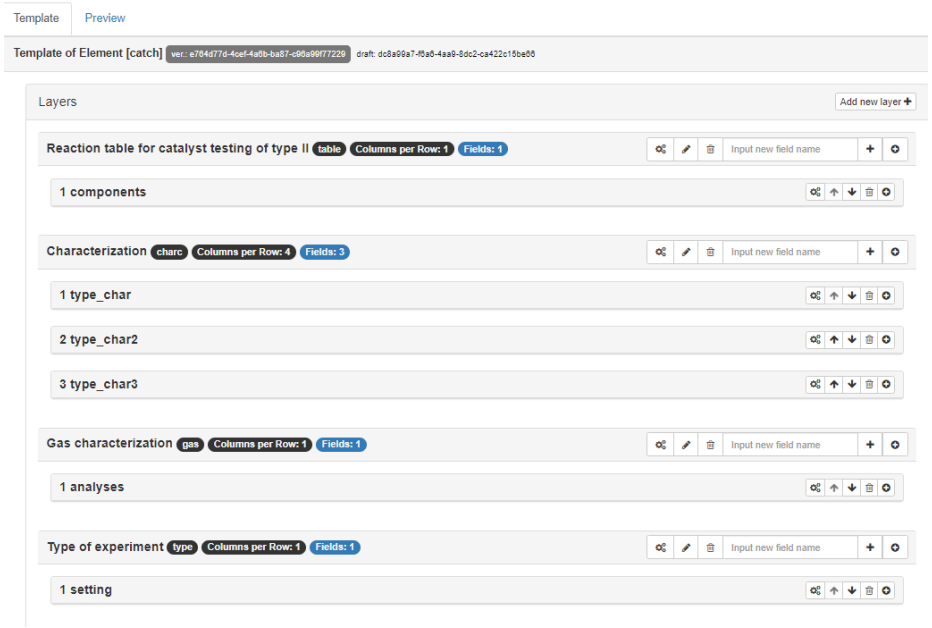
Chemotion - Basic view

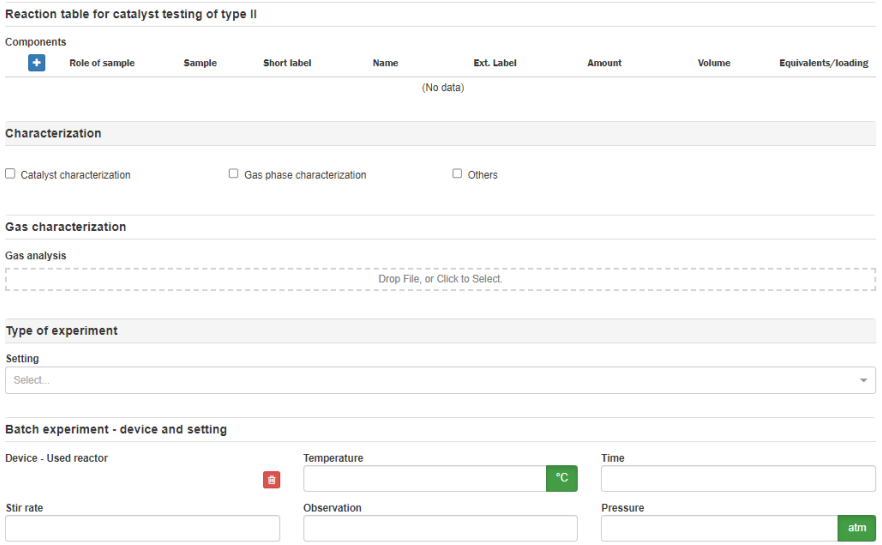


Chemotion - Generic Elements

- For non-synthetic workflows
- Create your own workflows

LabMotion





https://www.chemotion.net/docs/eln/admin/generic_config

Chemotion ELN: Analyze NMR data

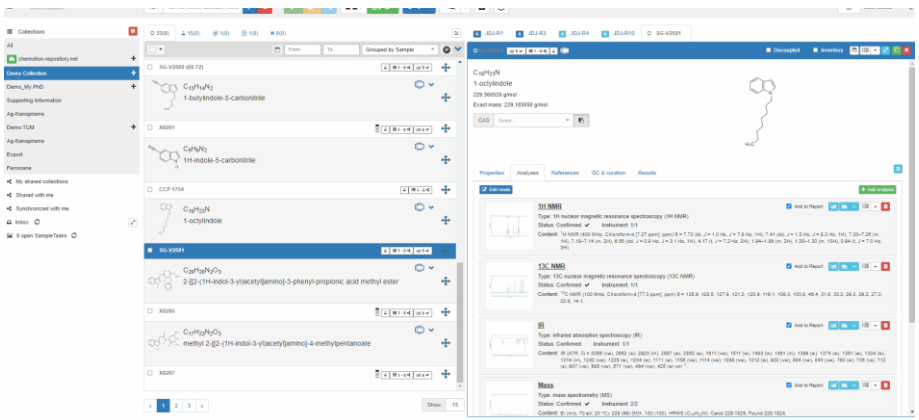
ChemSpectra for 1D NMR data

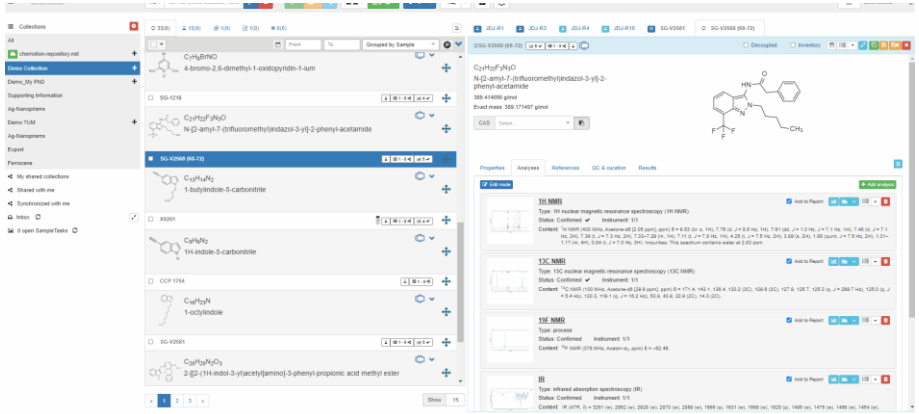
- Options to analyze data and store results back to ELN

NMRium integration for 1D and 2D NMR data

- NMRium: advanced NMR analysis (1D, 2D)

Interoperable



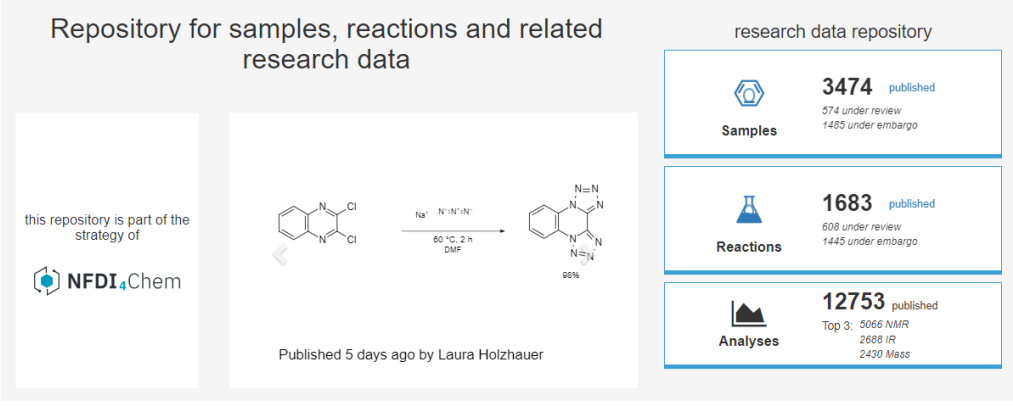


Publishing in the Chemotion Repository

- Collections, reactions and or samples can be published easily to the Chemotion Repository (Open Access)
- ChemConverter also implemented in Repository
- Among list of recommended repositories of Angewandte Chemie
- https://www.chemotion-repository.net/

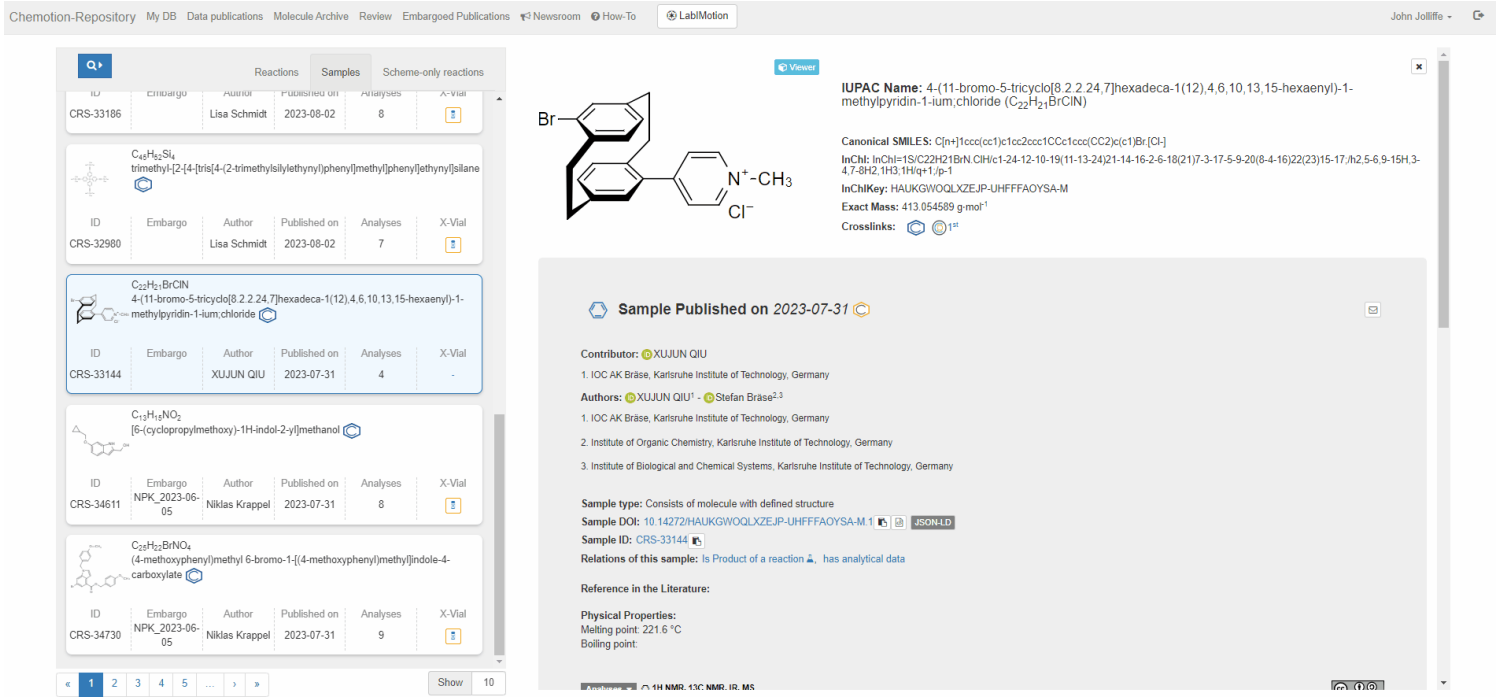
Chemotion Repository

https://t1p.de/b13zw

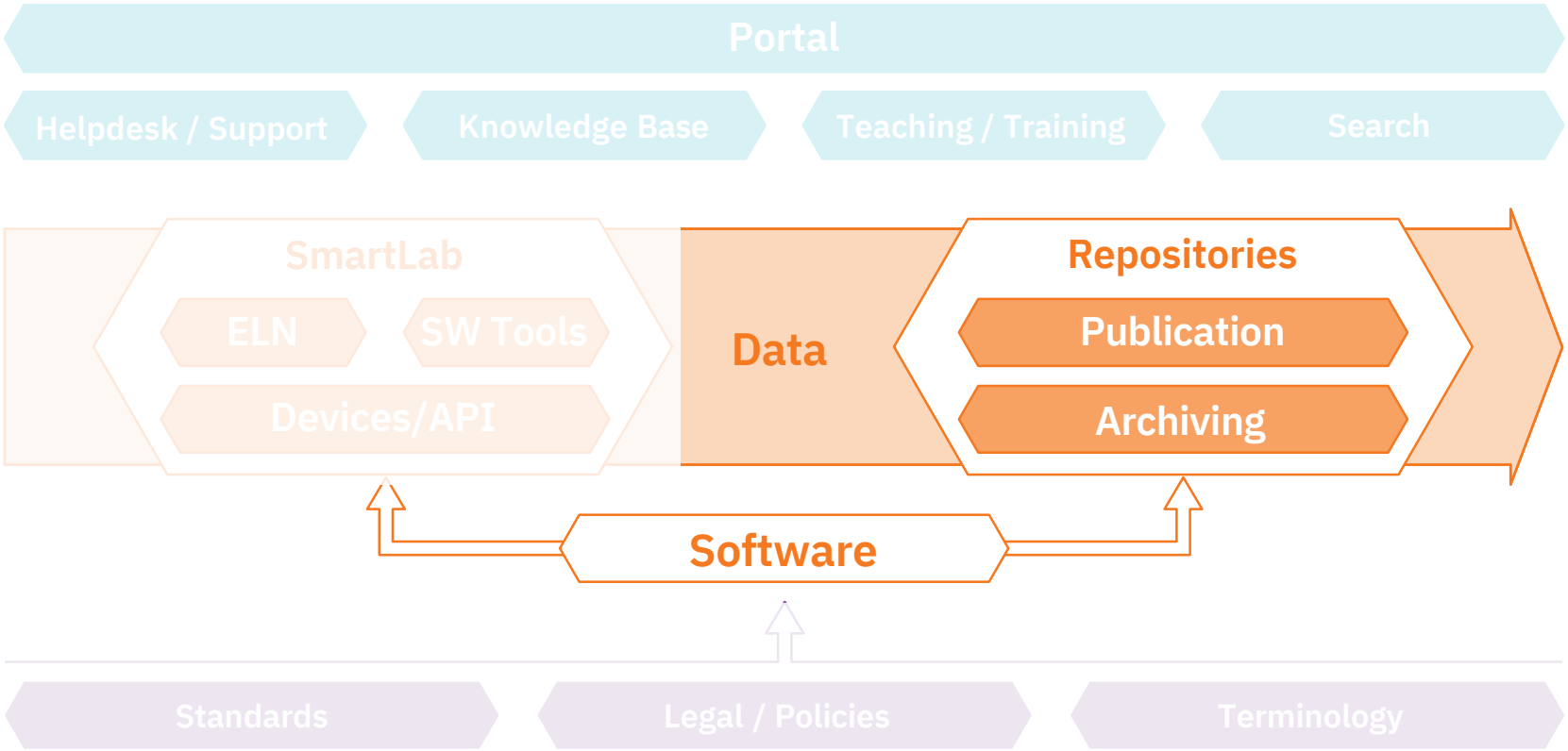


Data in the Chemotion Repository

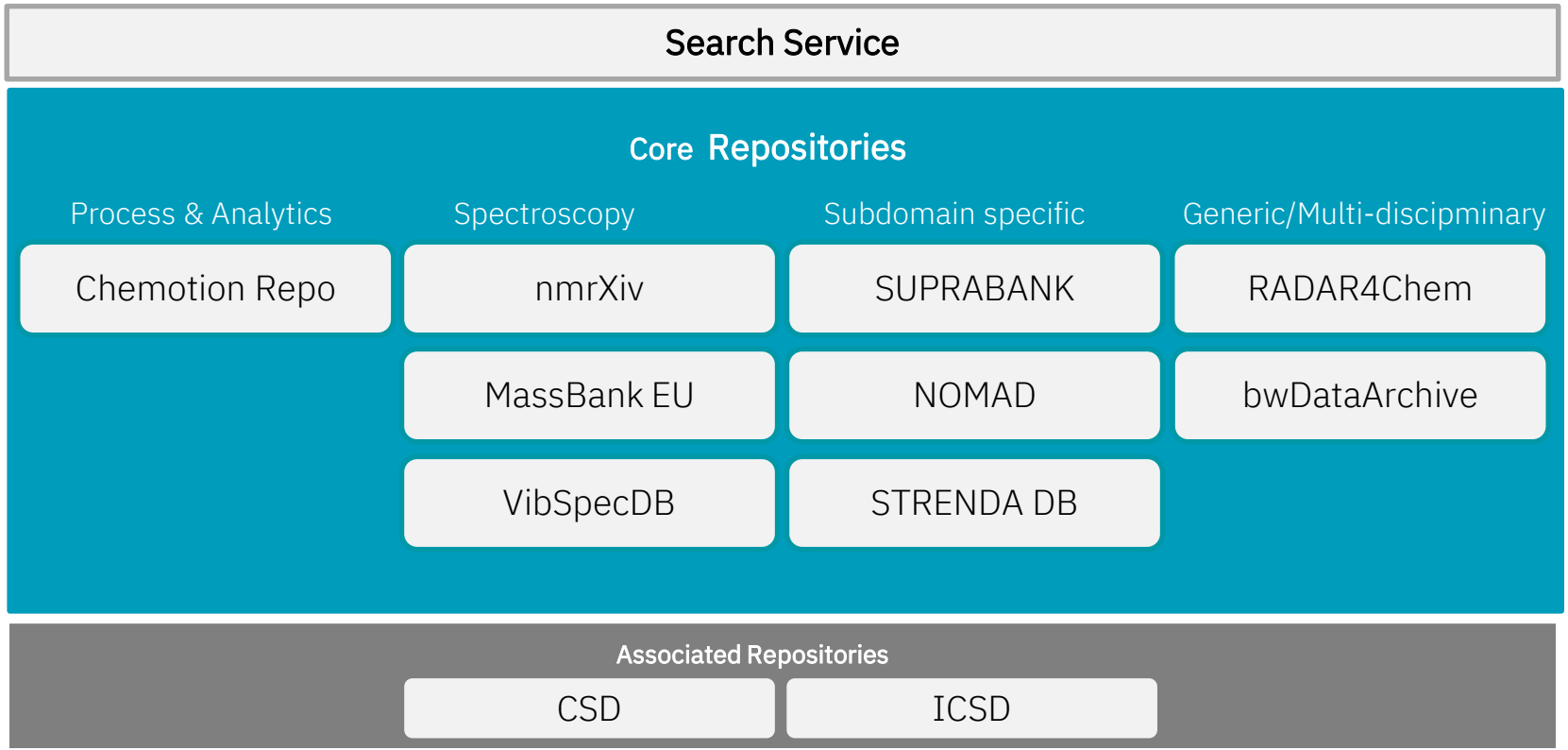
- Every reaction/sample & every analysis get their own DOIs
- Interact with spectra directly via the browser (no ELN necessary)



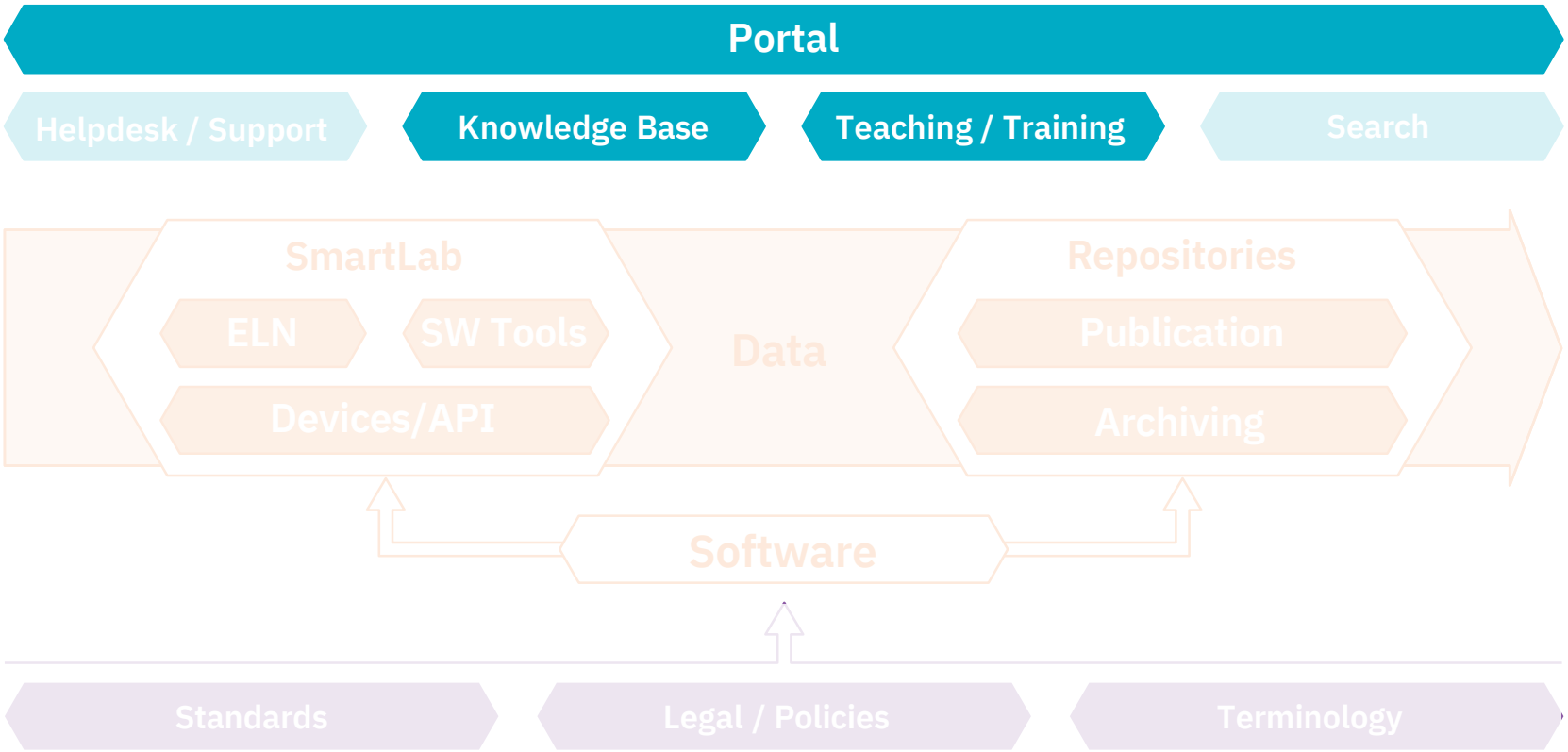
ELNs & Repositories



Federation of Repositories

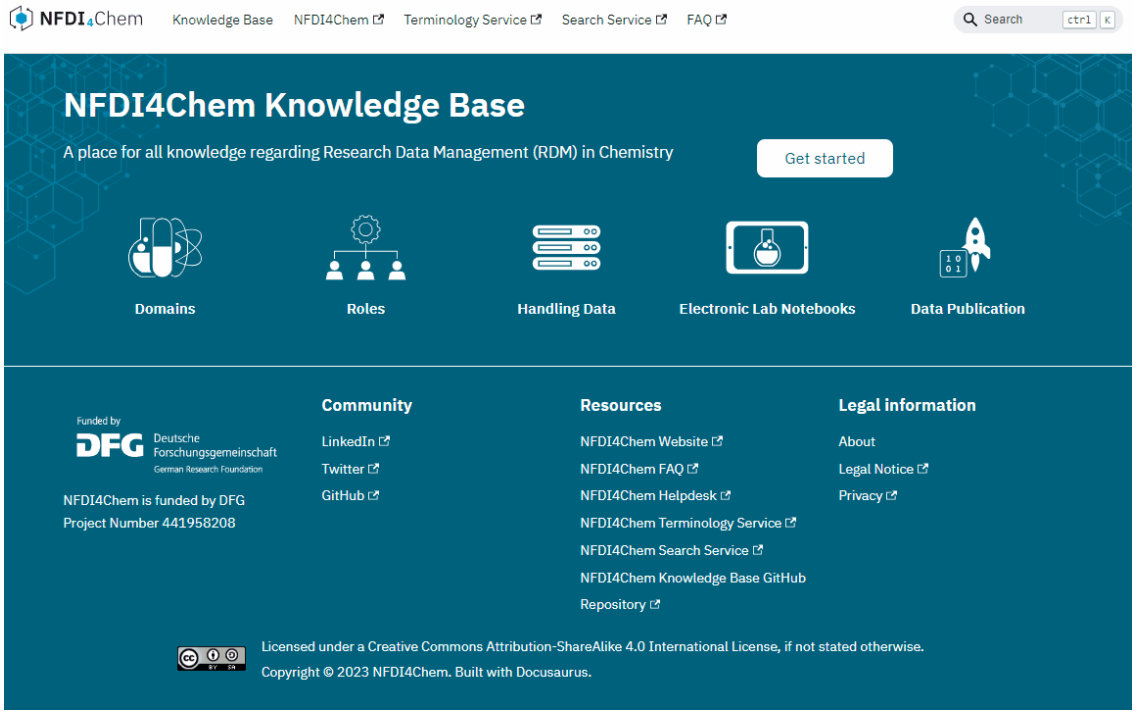


Knowledge Base



NFDI4Chem Knowledge Base

- Access to Research Data Management (RDM) knowledge via various points of entry



https://knowledgebase.nfdi4chem.de/

Digital Literacy in Undergraduate Degrees

GDCh Empfehlung: Kerncurriculum Bachelor Chemie, 2021

Inhalte Datenwissenschaften:

„Forschungsdatenmanagement: Unterscheidung zwischen Roh- und aufbereiteten Daten, gute wissenschaftliche Praxis im Kontext von Forschungsdaten; elektronische Laborbücher, Repositorien; Metadaten, Annotation, Ontologien; Datenmanagementpläne, Forschungsdateninfrastruktur; rechtliche und ethische Anforderungen“

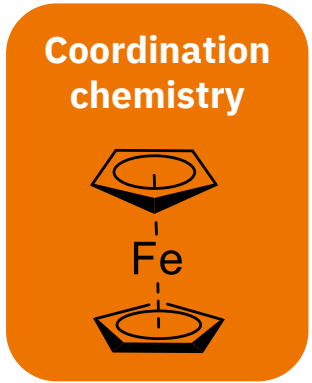
Survey 2023: 86 % of the participants think that RDM should be integrated into the curricula!

https://www.gdch.de/fileadmin/downloads/Service_und_Informationen/Downloads/Schule_Studium/PDF/2021_GDCh_Studienkommission_Druckversion.pdf

Framework

Advanced inorganic lab course for undergraduate students

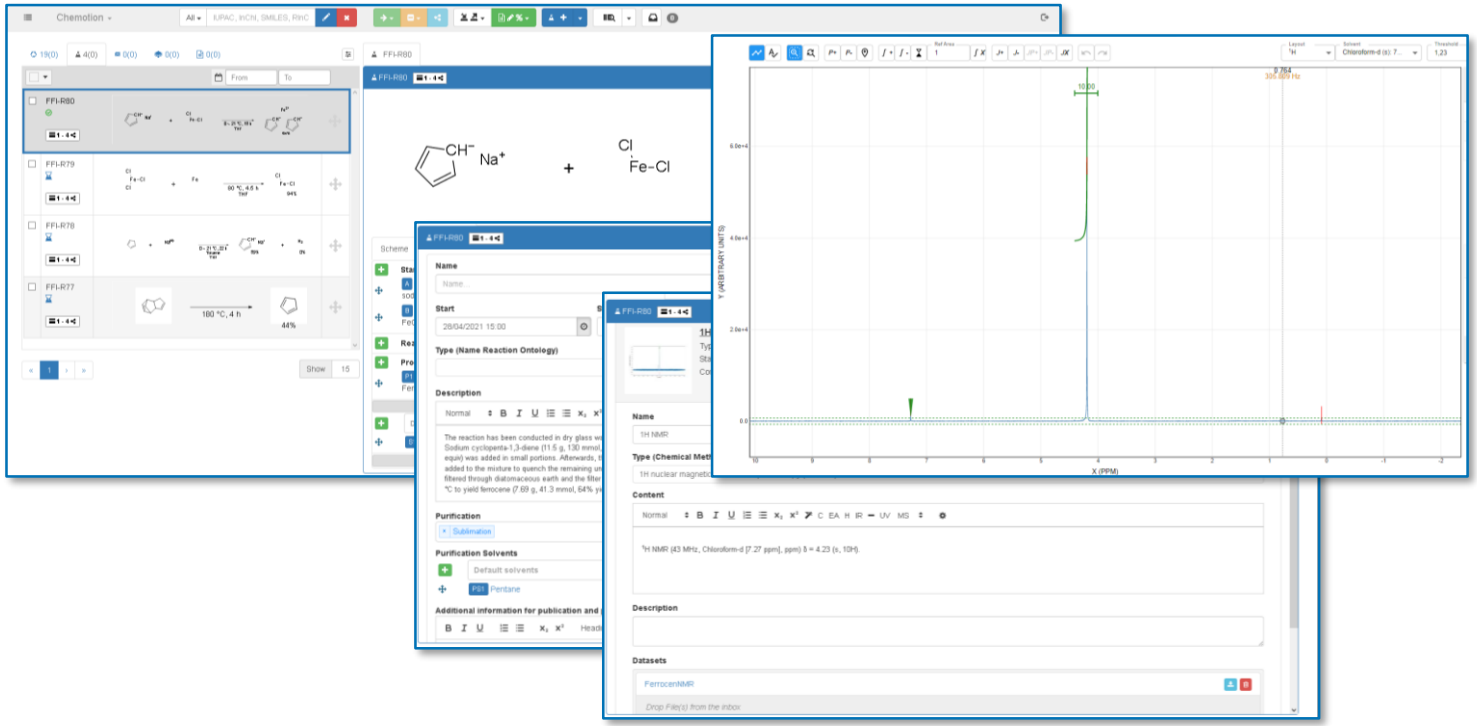
- Mandatory lab course for 5th semester bachelor students at RWTH Aachen
- Each winter term: 3 thematic blocks, 110 – 120 students
- Implementation of the Chemotion ELN (since WT20/21):
  - Synthesis of Ferrocene in the lab
  - Complete processing (planning, documentation, analysis) in the Chemotion ELN
- Learning unit on research data management (since WT20/21):
  - Short videos on the basics of RDM, FAIR principles, data management plans, metadata, and InChI & SMILES
  - Final test on RDM which students must pass in order to pass the lab course



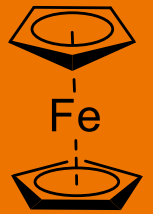
Chemotion

Digital Documentation in the ELN

Processing of the synthesis of Ferrocene in the Chemotion ELN



Coordination chemistry



J. Cheminform. **2017**, *9 (1)*, 54.

J. Cheminform. **2021**, *13 (1)*, 8.

Chem. Methods **2022**, *2 (10)*, e202200026.

Chemotion

RDM Workshops & Chemotion ELN Workshops

- Workshops for both Chemotion and chemistry-specific RDM
- Regular workshops online
- Institute specific workshops upon request
- **Until now: > 500 participants trained**

Data preservation

Funders & publishers: policies & requirements

FAIR

RDM

DMPs

Publishing

ELNs

Legal aspects

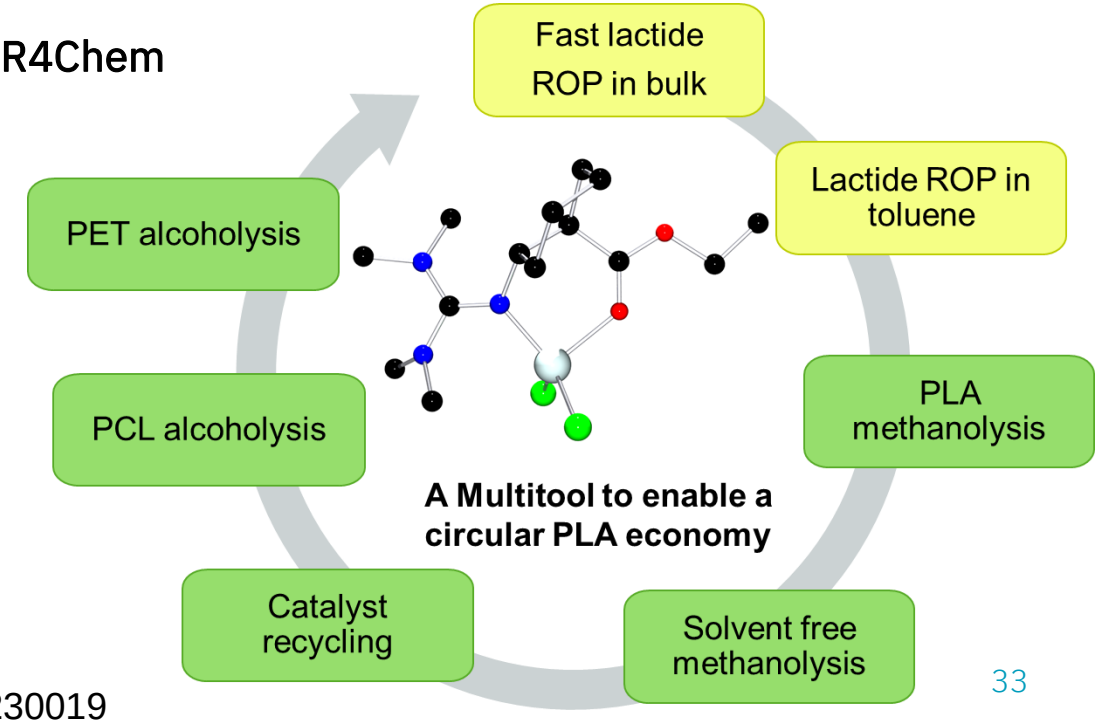
Data documentation

https://t1p.de/aw72j

Best Practices

- Example from ChemSusChem
- Synthetic data: **Chemotion Repo**
- Polymerisation kinetics etc: **RADAR4Chem**

- **Disciplinary examples and interdisciplinary examples**



SHP et al., *ChemSusChem* **2023**,*16*, e20230019

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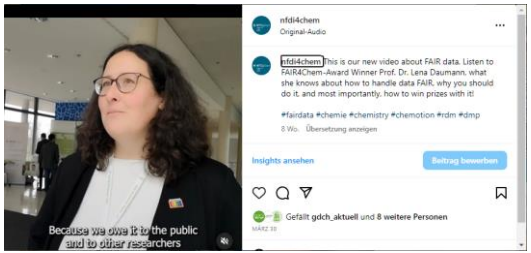

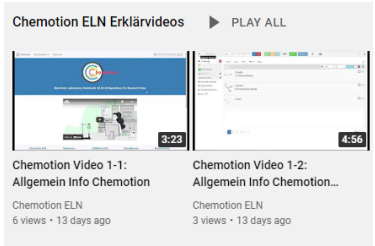

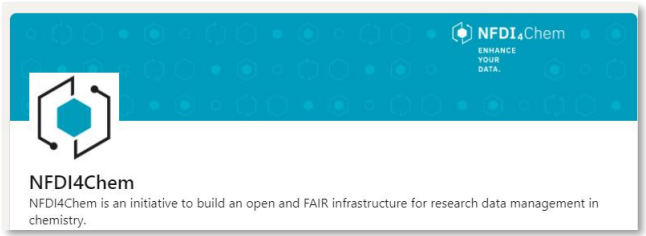

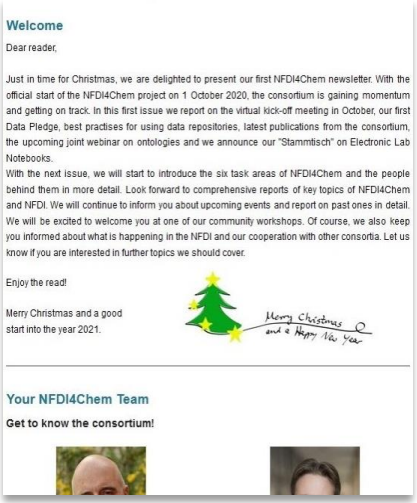

Thank you for Listening! – Any Questions?

Composition of the consortium

Ontologies4Chem Workshop