NFDI4Chem

ENHANCE
YOUR
DATA.

NFDI4Chem: Chemical Research Data Management and Digital Chemistry

Prof. Dr. Sonja Herres-Pawlis

March 23rd, 2022

National Research Data Infrastructure

Building a National Research Data Infrastructure:
Linking and enhancing existing infrastructure components by services

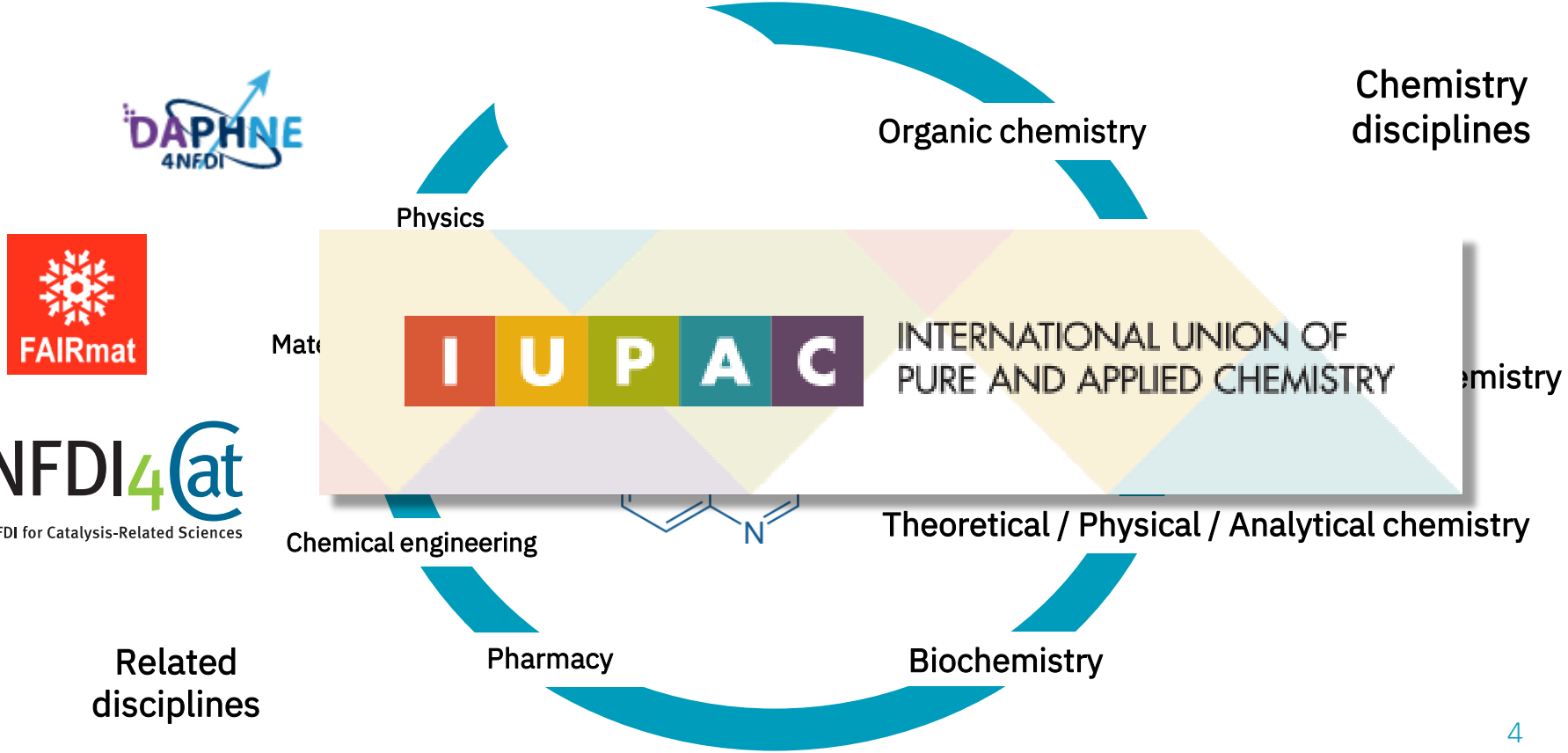
Numbers

- Up to **30 consortia** in NFDI representing sciences
- Community-driven process
- Funding of **€70m** per year in the final stage with 30 consortia.
- **~ €2.3m** per year for each consortium for 5 years (+5 years)
- Collaboration of all consortia in cross-cutting topics: Sections (4) and base services (~4)

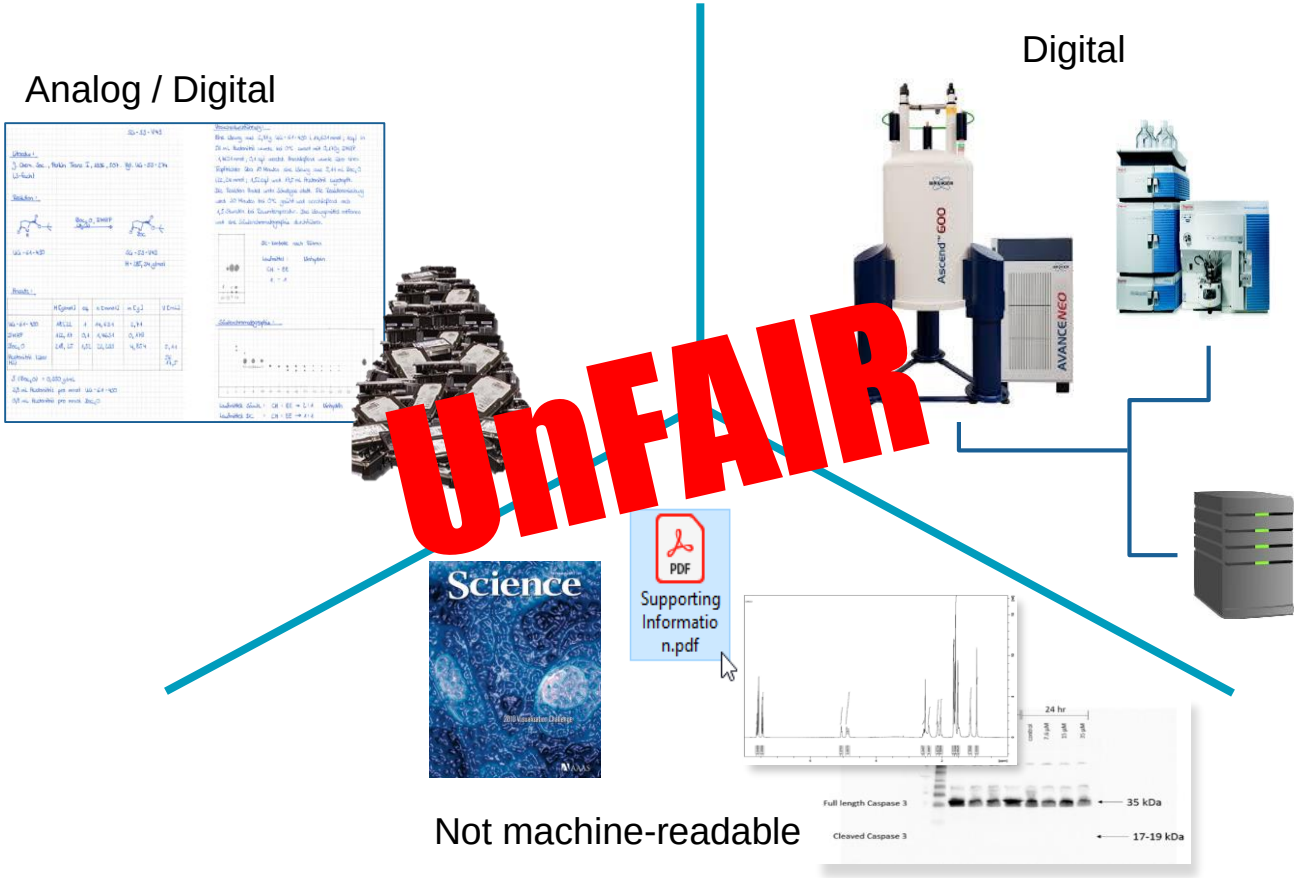
Introduction videos by DFG
https://www.youtube.com/watch?v=uJ01g9m8uE4
https://www.youtube.com/watch?v=qyKIfC1crjw

NFDI4Chem – Who we are

Our Scientific Community



Status Quo: Digital to Analog



Not machine-readable

Forces and Needs

n of a working group:

m 10 years ago?

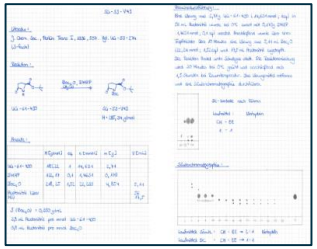
om 15 years ago?

made compound xy?

https://www.dfg.de/foerderung/info_wissenschaft/info_wissenschaft_22_25/index.html

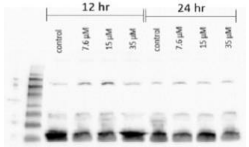
Our Focus: Molecules and Related Meta(data)

Reactions



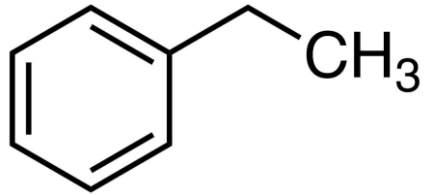
Experimental Description
Educts / Reagents
Conditions
...

Biological activity



Organism
Conditions
Activity
...

Properties



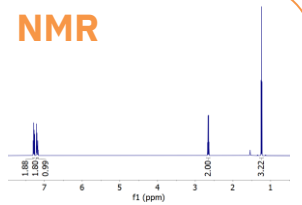
Name	Ethylbenzene
Formula	C_8H_{10}
CAS	100-41-4
InChI Key	YNQLUTRBYVCPMQ-UHFFFAOYSA-N

...

Spectra

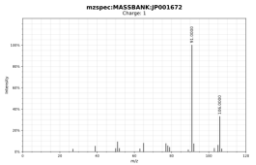
Assignment

NMR



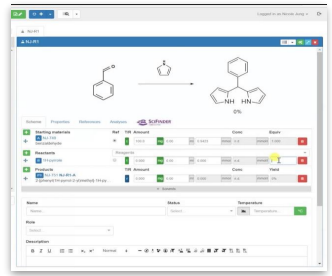
Nucleus
Pulse sequence
Solvent ...

MS



Ionisation method
Voltage ...

Our Vision



Digitalisation

Standards

Community

Re-use

Experiment Design

Experiment/ Data Collection

Data Processing

Analysis

Disclosure/ Publication

FAIR Data

Electronic Lab Notebooks

Repositories

Common Standards

NFDI4Chem Services

Legally reliable framework of policies and guidelines for FAIR research data management

- Recommendations for data and metadata standards with international bodies
- Development of Minimum Information of Chemical Investigations (MIChI)

- Training, Workshops & Roadshows
- Knowledge Base, Helpdesk
- Teaching Materials
- Flaghsip Labs, Best Practices

- Joining forces with publishers & editors
- RDM Recommendations
- RDM Author Guidelines

- Semantification of Data
- Terminology Service
- Development & Curation of Ontologies

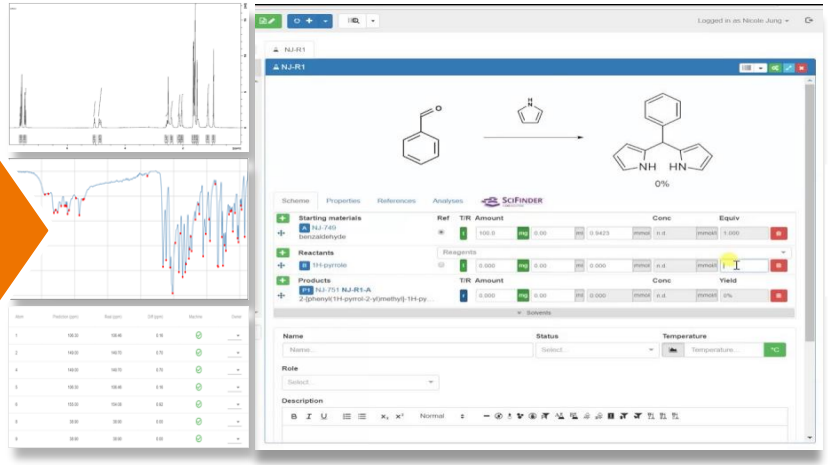
- Federation of Repos
- Applying FAIR Data
- MIChI

Smart Lab - Seamless Data Flows

Devices

Data

Electronic Lab Notebook (ELN)

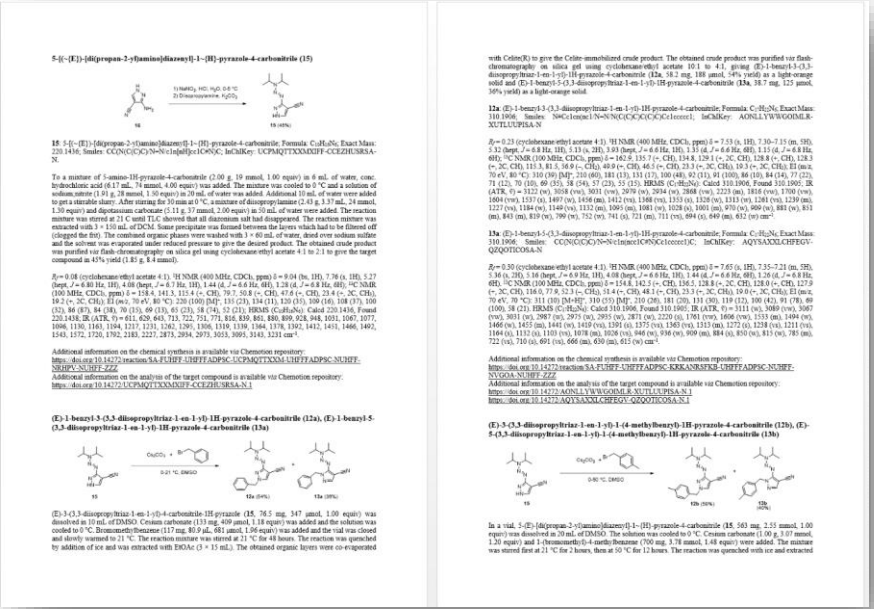


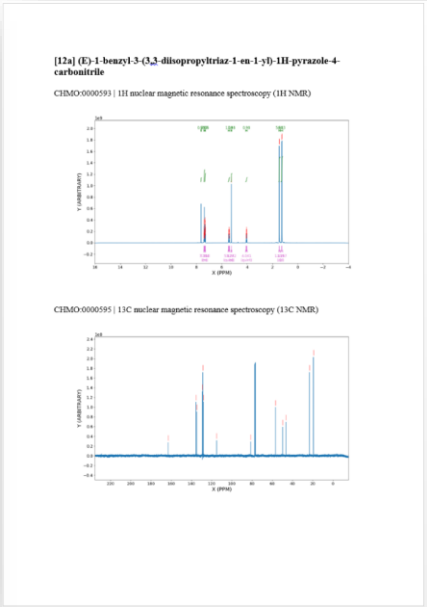
Data

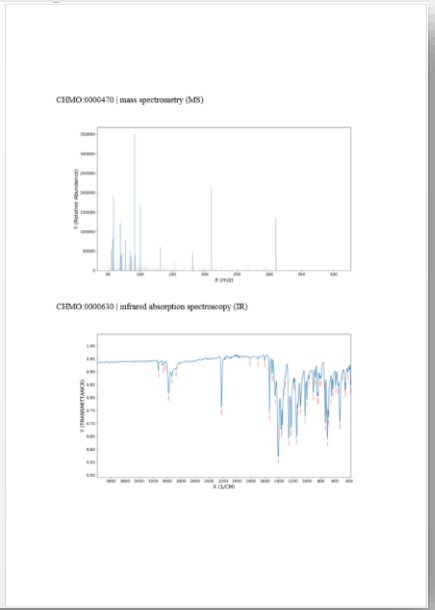
Federated Repositories

Chemotion ELN

ELN reporting function to generate SI

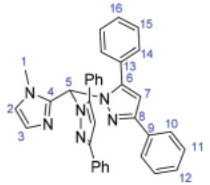






Synthesis of new pyrazolo[1,2,3]triazines by cyclative cleavage of pyrazolo-triazenes, Nicolai Wippert, Martin Nieger, Claudine Herlan, Nicole Jung and Stefan Bräse. *Beilstein Journal of Organic Chemistry*, preprint 2021.

Best practice



^{1}H NMR (CD_2Cl_2, 400 MHz): δ = 7.80 (d, ^{3}J = 7.8 Hz, 4H, H-10), 7.67 (s, 1H, H-5), 7.39 (t, ^{3}J = 7.4 Hz, 4H, H-11), 7.32 (d, ^{3}J = 7.3 Hz, 4H, H-12 + H-16), 7.27 (t, ^{3}J = 7.3 Hz, 4H, H-15), 7.12 (d, ^{3}J = 7.1 Hz, 4H, H-14), 6.94 (d, ^{3}J = 3.1 Hz, 2H, H-2 + H-3), 6.65 (s, 2H, H-7), 3.70 (s, 3H, H-1) ppm. **^{13}C {^{1}H} NMR (CD_2Cl_2, 100 MHz):** δ = 151.8 (C-8), 146.4 (C-6), 142.5 (C-4), 133.7 (C-9), 129.5 (C-13), 129.4 (C-14), 129.1 (C-15), 129.1 (C-12 + C-16), 128.5 (C-11), 128.0 (C-3), 126.3 (C-10), 124.3 (C-2), 106.3 (C-7), 70.0 (C-5), 34.9 (C-1) ppm. **HRMS (ESI^{+}, MeOH):** *m/z* (found) = 533.24353 (100%), 534.24664 (37%), 535.25024 (7%), 536.25299 (1%); *m/z* (calc.) = 533.24537 (100%, $^{12}C_{35}{}^{1}H_{29}{}^{14}N_6{}^{+}$), 534.24872 (38%, $^{12}C_{34}{}^{13}C^{1}H_{29}{}^{14}N_6{}^{+}$), 535.25207 (7%, $^{12}C_{33}{}^{13}C_2{}^{1}H_{29}{}^{14}N_6{}^{+}$), 536.25543 (1%, $^{12}C_{32}{}^{13}C_3{}^{1}H_{29}{}^{14}N_6{}^{+}$). **IR (ATR, neat), $\tilde{\nu}$ [cm^{-1}]:** 1605 (vw), 1551 (w), 1459 (w), 1437 (w), 1410 (vw), 1298 (vw), 1281 (vw), 1259 (w), 1202 (w), 1138 (vw), 1076 (w), 1027 (w), 1007 (w), 957 (w), 916 (w), 868 (w), 841 (w), 834 (w), 816 (m), 803 (w), 767 (m), 759 (vs), 752 (s), 704 (m), 691 (vs), 678 (m), 666 (m), 573 (m), 524 (w), 432 (vw).

Additional information on the NMR of the target compound including original data files is available *via* Chemotion Repository: https://dx.doi.org/10.14272/LSGGPBYVWWQPOY-UHFFFAOYSA-N.1

Dalton Transactions

PAPER

Check for updates

Cite this: DOI: 10.1039/d1dt00832c

https://www.chemotion-repository.net/welcome

ROYAL SOCIETY OF CHEMISTRY

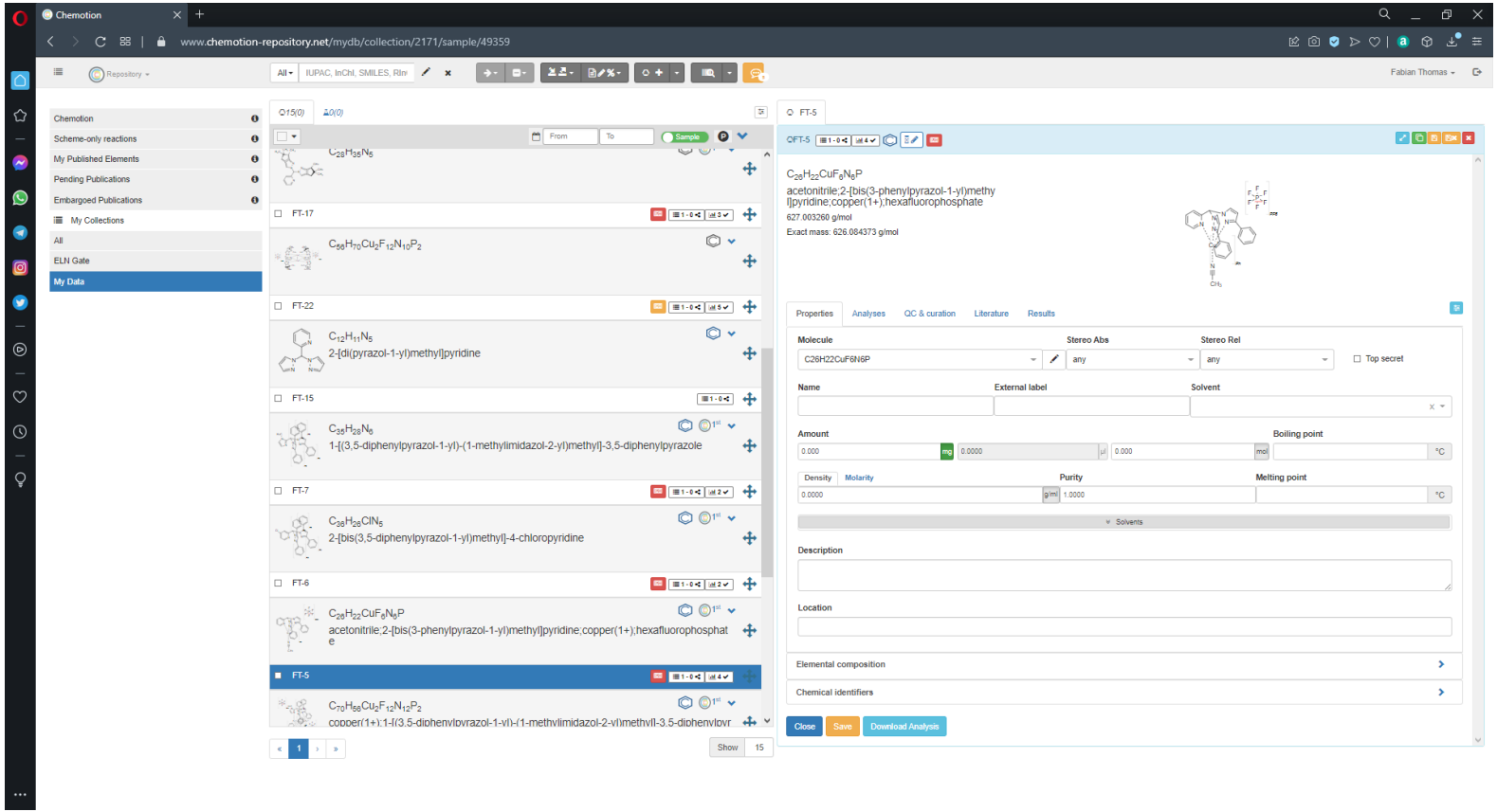
View Article Online
View Journal

A … pper nitrenes and … amination

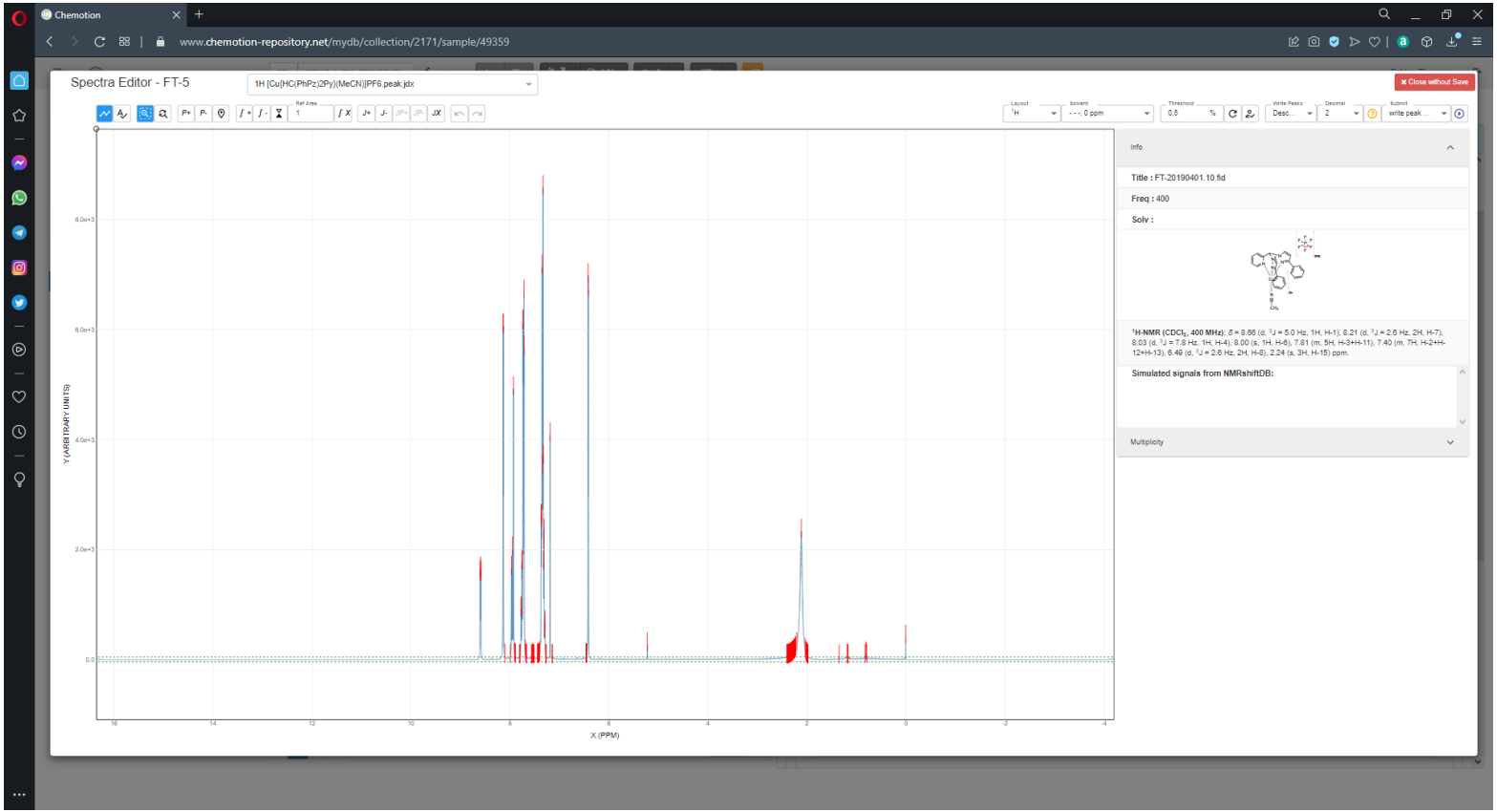
… ai C. Göbgen, … mann … and

… as intermediates in the copper cata- … complexes were synthesized at low … pyrazolyl)methane family. The copper nitrenes were obtained by the reaction of a copper(I) acetonitrile complex with ^{S}PhINTs in dichloromethane.

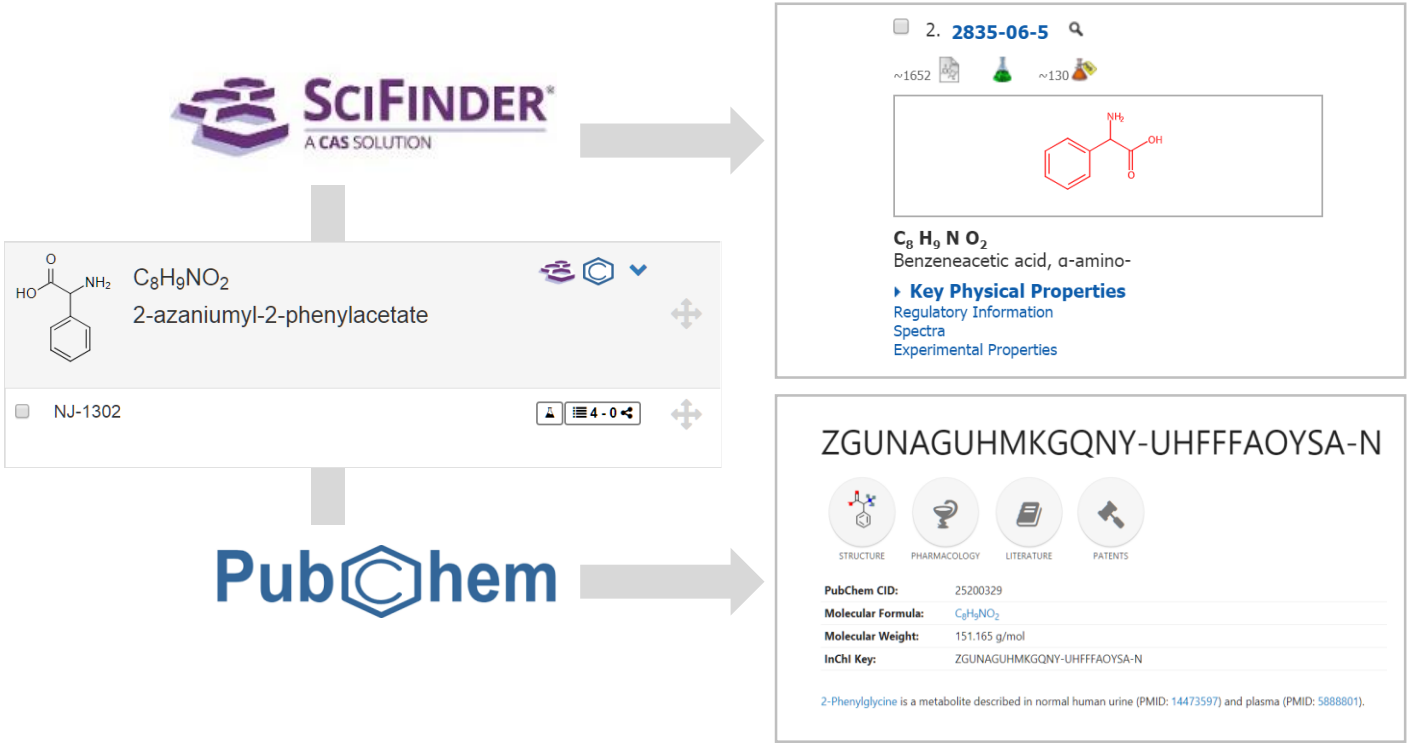
Chemotion Repo



Chemotion Repo



Chemotion Repo – Connection to Other Databases



Further Repos

- Hosted at FIZ Karlsruhe
- Free for the community
- All data welcome
- With generated doi and full metadata

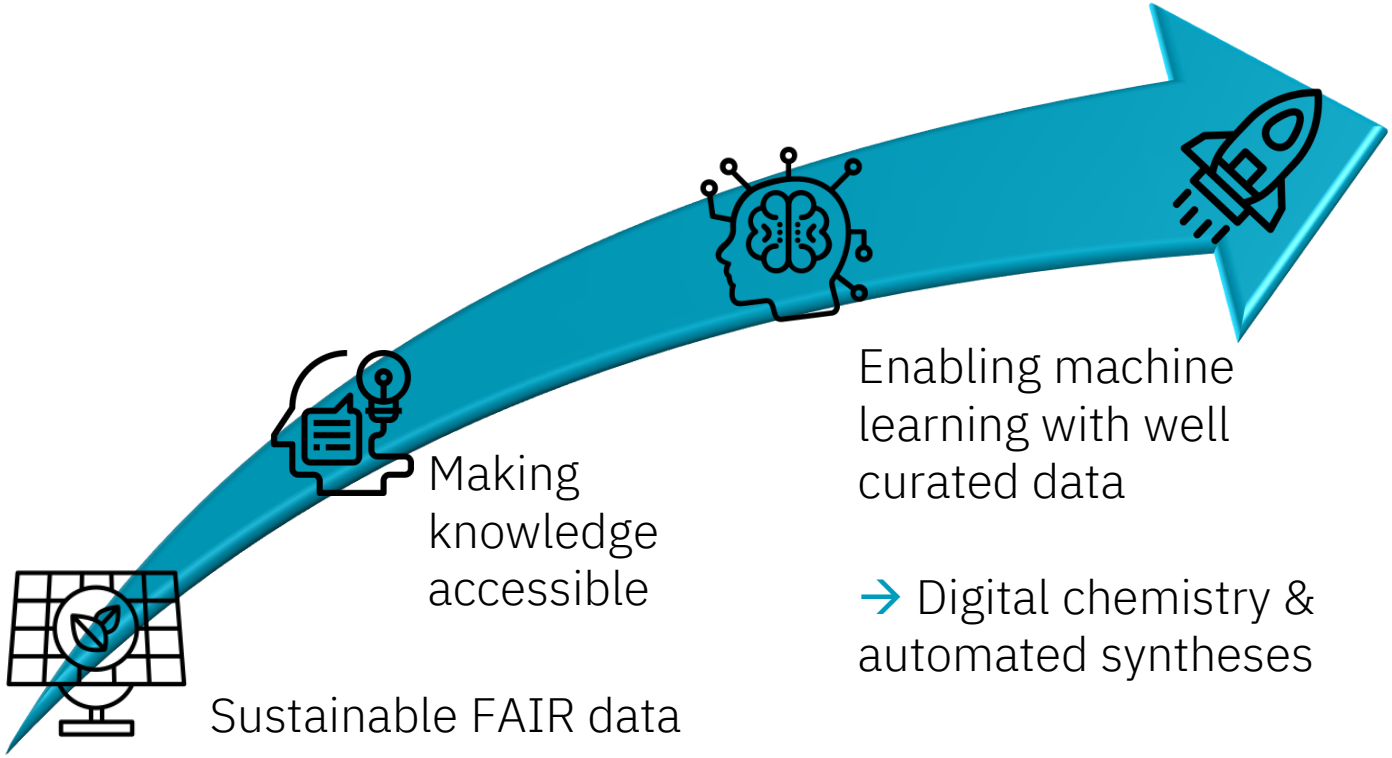
https://radar.products.fiz-karlsruhe.de/de/radarabout/radar4chem

- Hosted at FSU Jena
- Free for the community
- NMR data welcome
- With generated doi and full metadata
- Direct transfer from Chemotion ELN

https://docs.nmrxiv.org/

[We are actively working on the platform and content changes are expected.]

On the way to digital chemistry



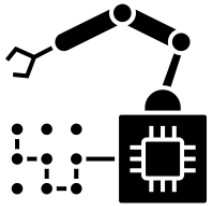
Sustainable FAIR data

Making knowledge accessible

Enabling machine learning with well curated data

→ Digital chemistry & automated syntheses

Accelerating research



Involvement of the Community

Community requirements

RDM
Infrastructure

Fostering cultural change

Raising RDM awareness

Involvement of the Community

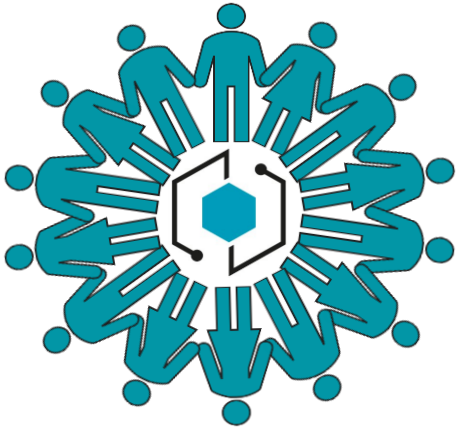
Newsletters

Website

Social Media

Local Helpdesks

Requirement Analysis



Workshops

Training

Tutorials

Roadshows

RDM Ambassadors

Best Practice

Flagship Labs

Curricular Embedding

Teaching Materials

Involvement of the Community

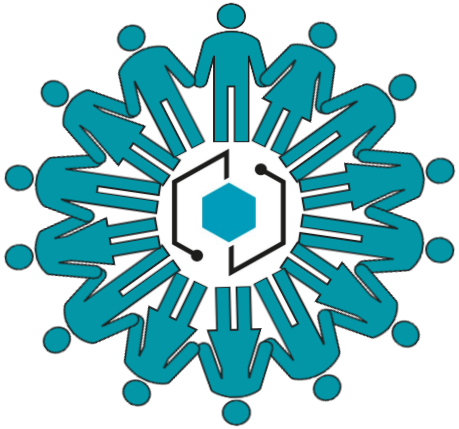
Newsletters

Website

Social Media

Local Helpdesks

Requirement Analysis



Workshops

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Curricular Embedding

Teaching Materials

Curricular Embedding:
Data Literacy in Undergraduate Degrees

Curricular recommendations of GDCh:

- **Published in September 2021**
- Anchoring data literacy and research data management modules already in the B.Sc. studies
- BUT: long way through the institutions…

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

Integration into Curricular Teaching – Example 1

Faster way: Pre-integration into content of running lectures

Example 1: Master lecture Sustainable coordinative polymerisation catalysis

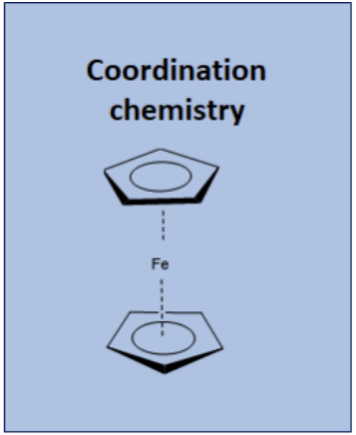
- Optional lecture (2h per week) in the master studies @RWTH
- 80-100 students, 50 take the exam
- Explaining chemistry with case studies
- Dissecting the RDM of the case studies (good and bad examples)
- Integrating videos on the basics of RDM from RWTH library/NFDI4Chem

Integration into Curricular Teaching – Example 2

Faster way: Pre-integration into content of running lectures

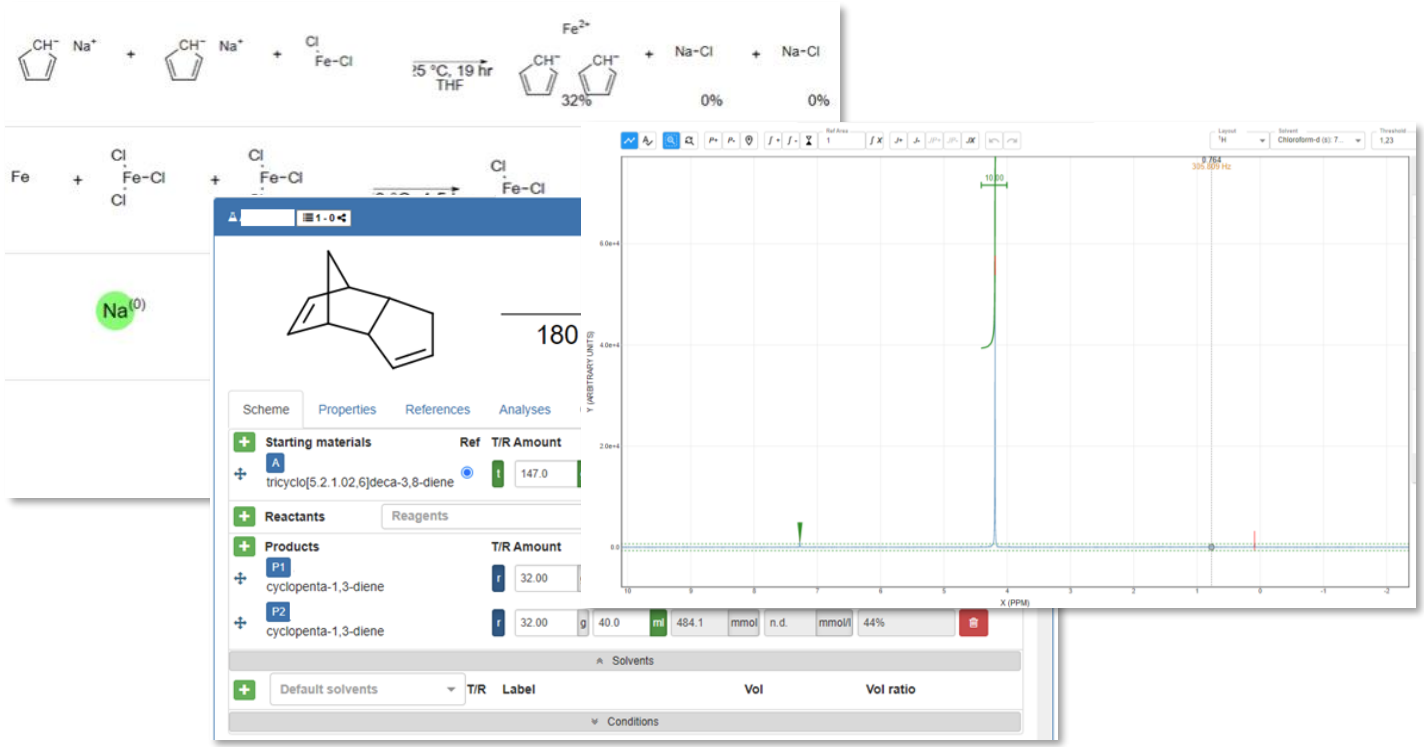
Example 2: Lab stage in Advanced inorganic chemistry

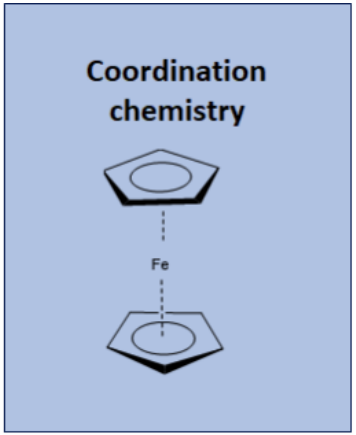
- 5th semester in bachelor studies @RWTH
- ~130 students
- Introduction to the Electronic Laboratory Notebook Chemotion
- Integrating videos on the basics of research data management, FAIR principles, data management plans, metadata and InChI & SMILES
- Self practice: Synthesis of Ferrocene, complete processing in Chemotion ELN



Integration into Curricular Teaching – Example 2

Processing of the synthesis of Ferrocene in Chemotion ELN:





Teaching for Chemotion

Chemotion teaching materials

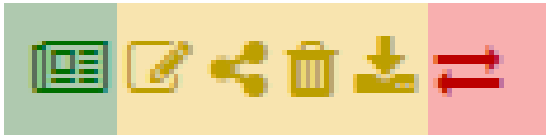
- Training/support for researchers on all levels: https://chemotion.net/chemotionsaurus/docs/category/manual
- Training videos for beginners and advanced users: https://zenodo.org/record/6356844#.YjDgfTUxlPZ

Chemotion roadshows

- Members of our Chemotion team visit you on site or virtually for an in-depth introduction and answer generic and specific questions: https://www.nfdi4chem.de/index.php/chemotion-roadshows/

Guidelines for Sharing in Chemotion

- Chemotion working group policy as applied by a synthesis-oriented working group: DOI: 10.26434/chemrxiv-2022-t4p5n
- Allows to set up a group database and to structure the data sharing within different permission levels indicated by six pictograms.



Workshop: FAIR RDM: Basics for Chemists

Costs: Free

Venue: Online

Duration: 2 days, 4-6 hours each

Participants: ~ 20 per Workshop

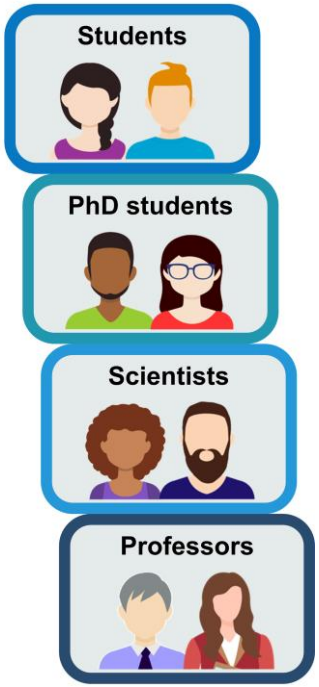
Registration: https://www.nfdi4chem.de/

#	Day 1	Day 2
2	20.04.2022	22.04.2022
3	22.06.2022	24.06.2022
4	17.08.2022	19.08.2022
5	19.10.2022	21.10.2022
6	07.12.2022	09.12.2022

Upon request, in-person workshops at institutions

More Chemistry-specific Roadshows/Webinars

for all career stages:

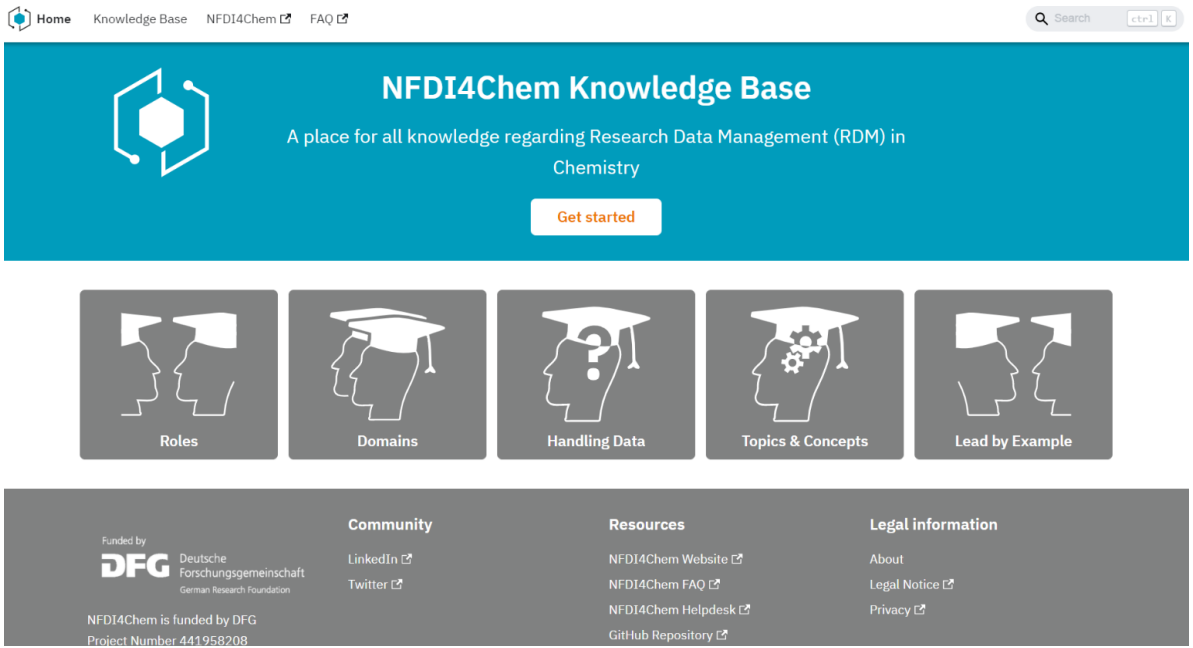


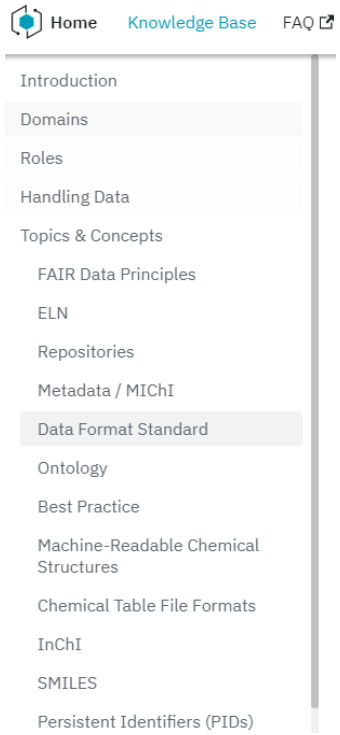
- NFDI4Chem to give general **talks about the consortium and RDM** virtual/throughout the country
- **Chemotion/NFDI4Chem Stammtisch** last Friday every month: **03/25 @ 2 p.m.** ***Modern RDM in Chemistry***
- **Chemotion ELN Q&A Session** every second Thursday (introductions/questions/get help): **03/24 @ 3 p.m.**

Registration via **https://www.nfdi4chem.de/**

Knowledge Base

https://knowledgebase.nfdi4chem.de/knowledge_base/





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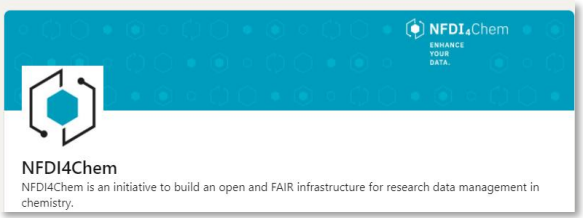

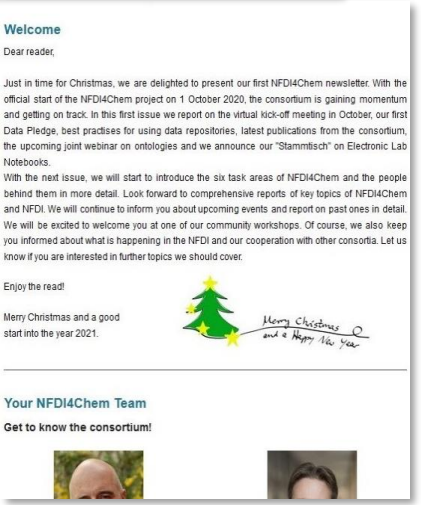

Subscribe to our newsletter which is released every quarter!

Christoph Steinbeck*
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Johannes Liermann
Johannes Gutenberg University Mainz

Oliver Koepler*
TIB Leibniz Information Centre of Science and Technology

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NFDI4Chem

ENHANCE YOUR DATA!

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