



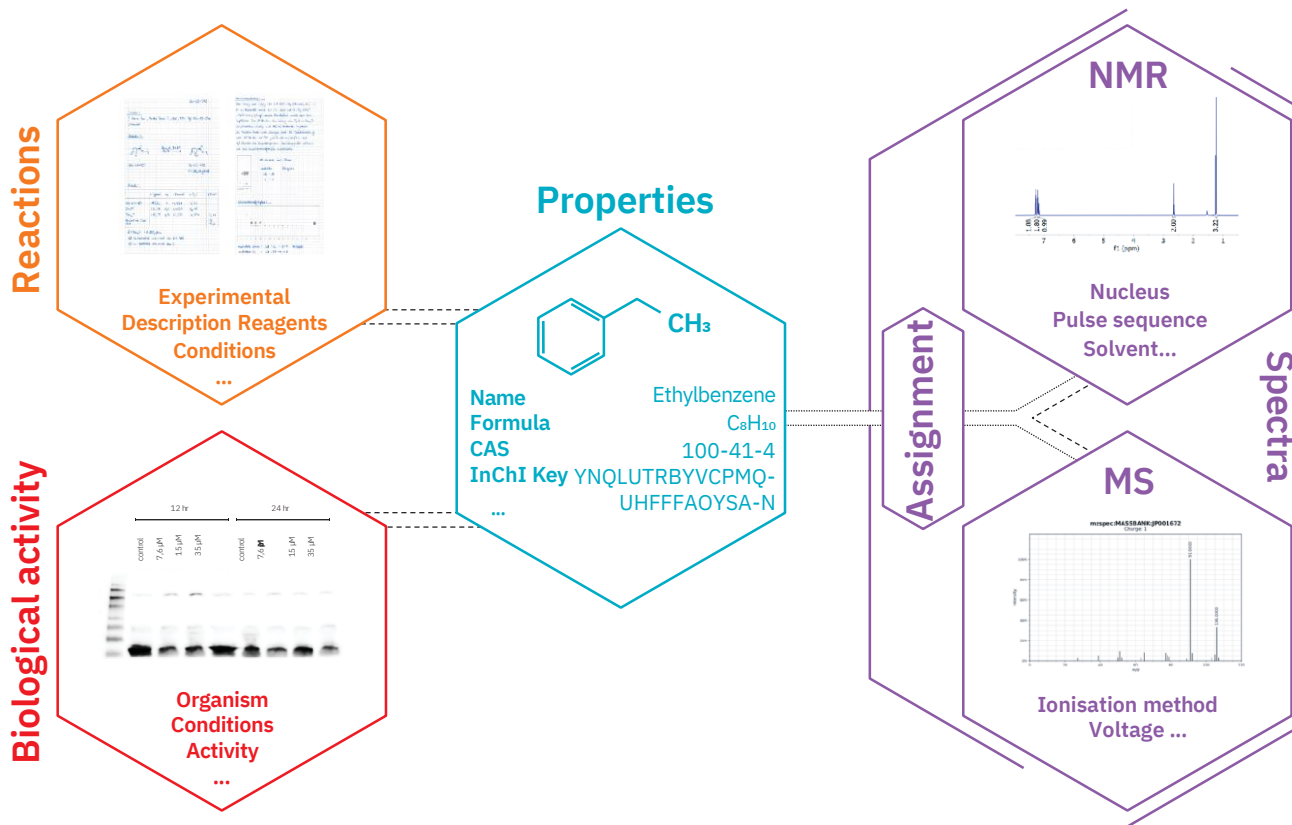
NFDI₄Chem

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)

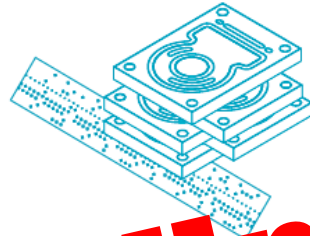


Status Quo



Analogue / Digital

The image shows a page from a scientific document or lab notebook. It contains handwritten text, chemical structures, and tables of data. The text is in German and appears to be a protocol or report. There are several tables with columns and rows of numbers and text. The overall appearance is that of a physical document, not a digital file.

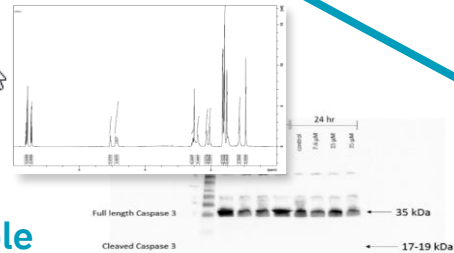
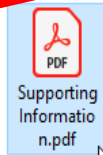
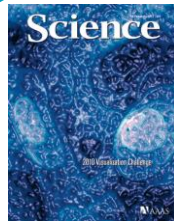


Digital



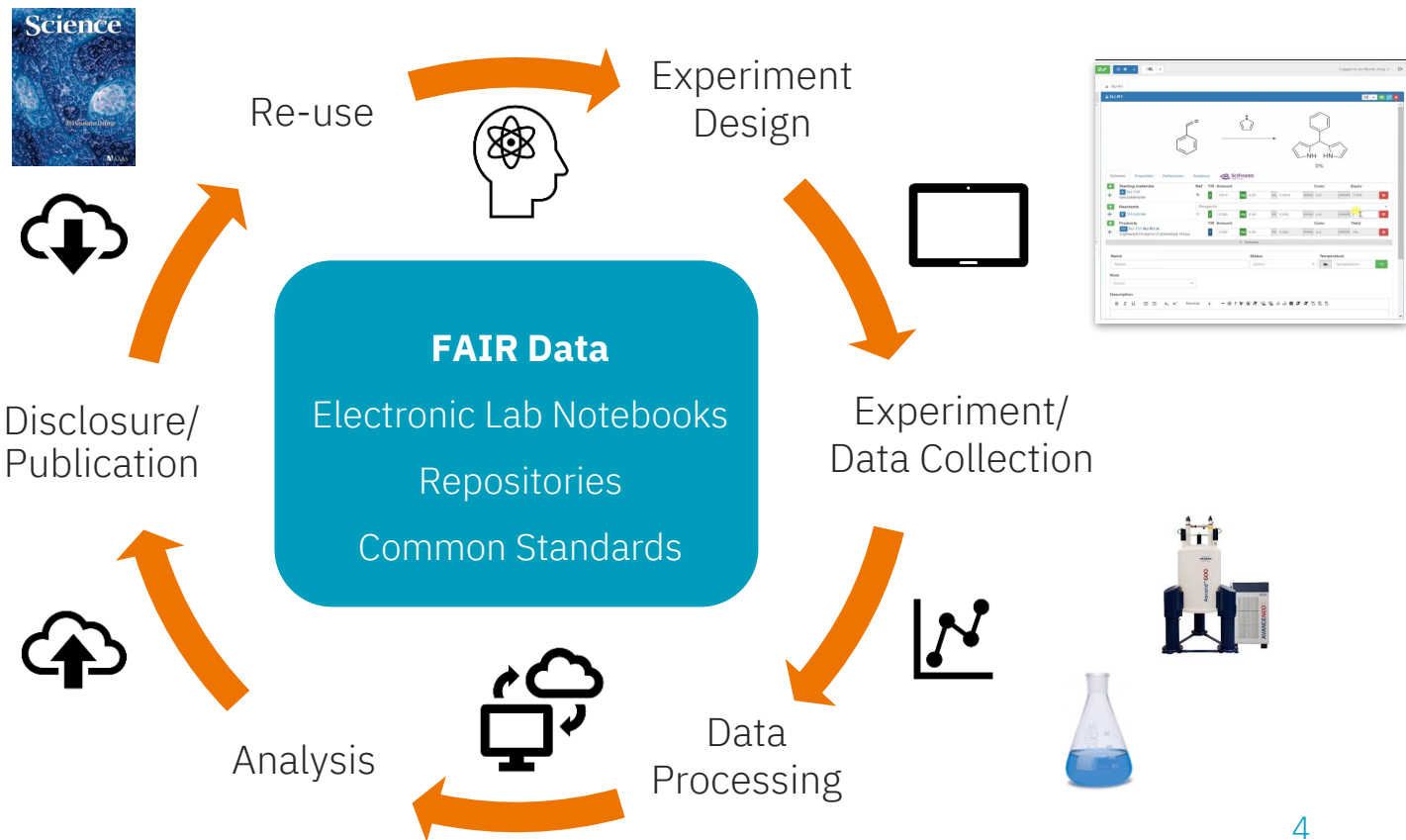
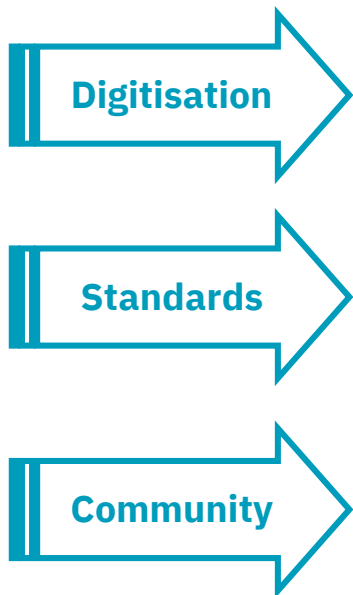
UnFAIR

Findable
Accessible
Interoperable
Reusable



Not machine readable

Our Vision





NFDI₄Chem

ENHANCE
YOUR
DATA.

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



VS.



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



- 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**

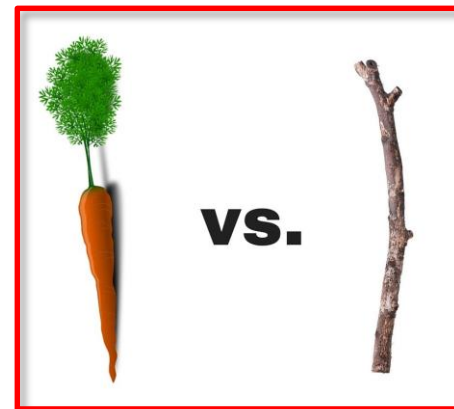
EDITORS
4Chem 

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
- 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

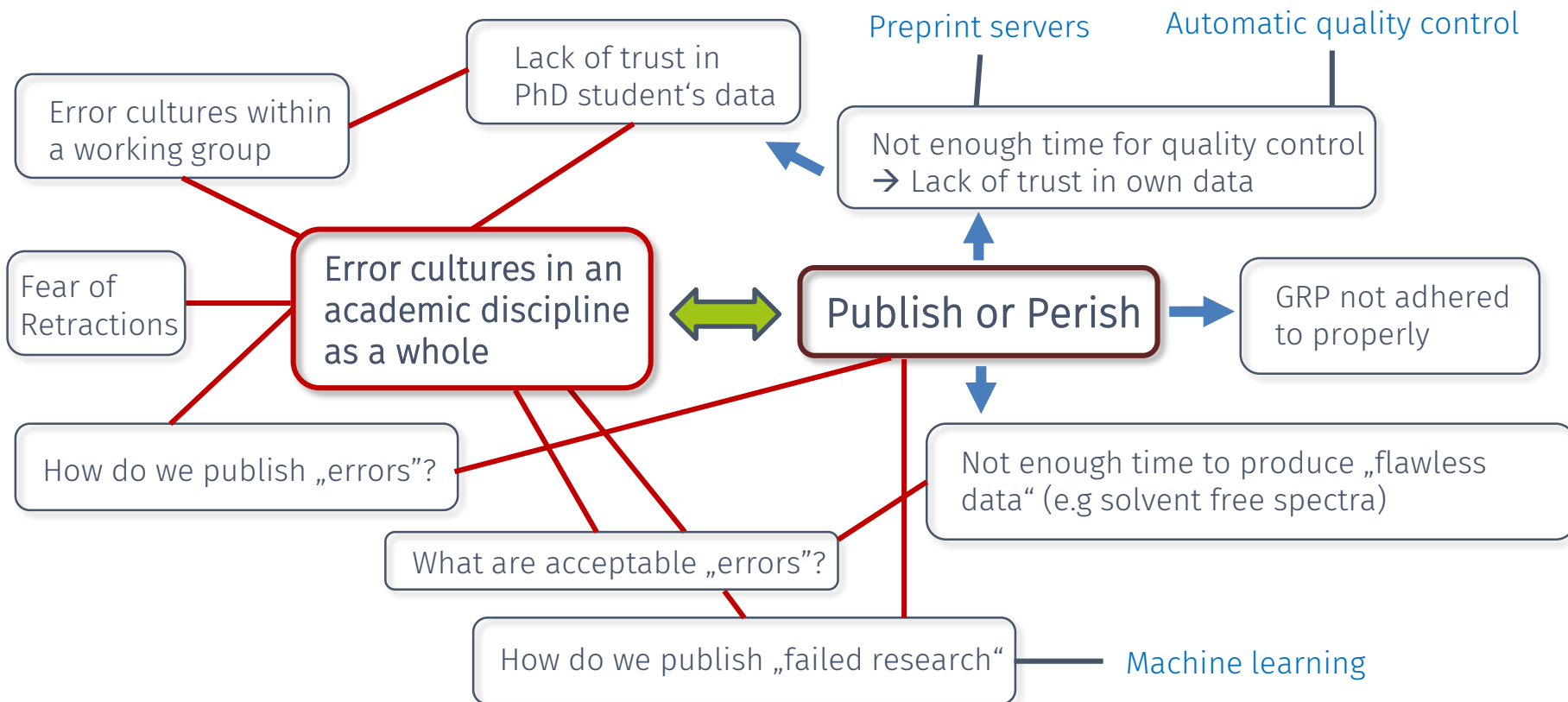


Why is there are reluctance to publish data?



„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.



NFDI₄Chem

ENHANCE
YOUR
DATA.

What do we offer?

ELNs & Repositories



Portal

Helpdesk / Support

Knowledge Base

Teaching / Training

Search

SmartLab

ELN

SW Tools

Devices/API

Data

Repositories

Publication

Archiving

Software

Standards

Legal / Policies

Terminology

Smart Lab - Seamless Data Flows

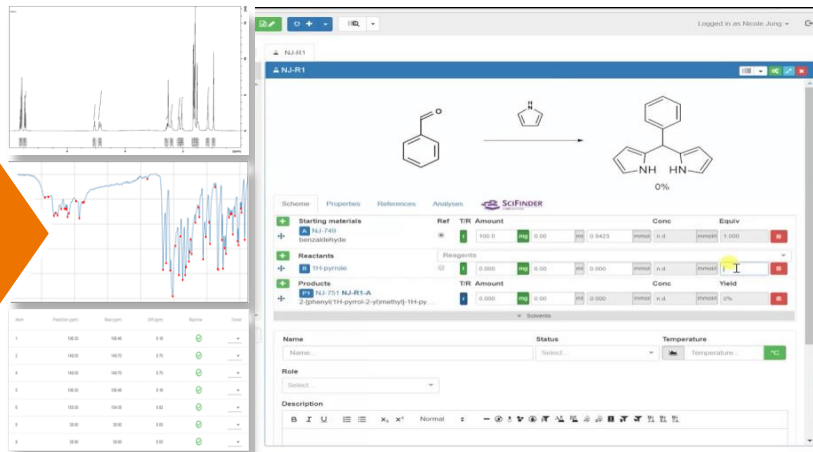


Devices



Data

Electronic Lab Notebook (ELN)



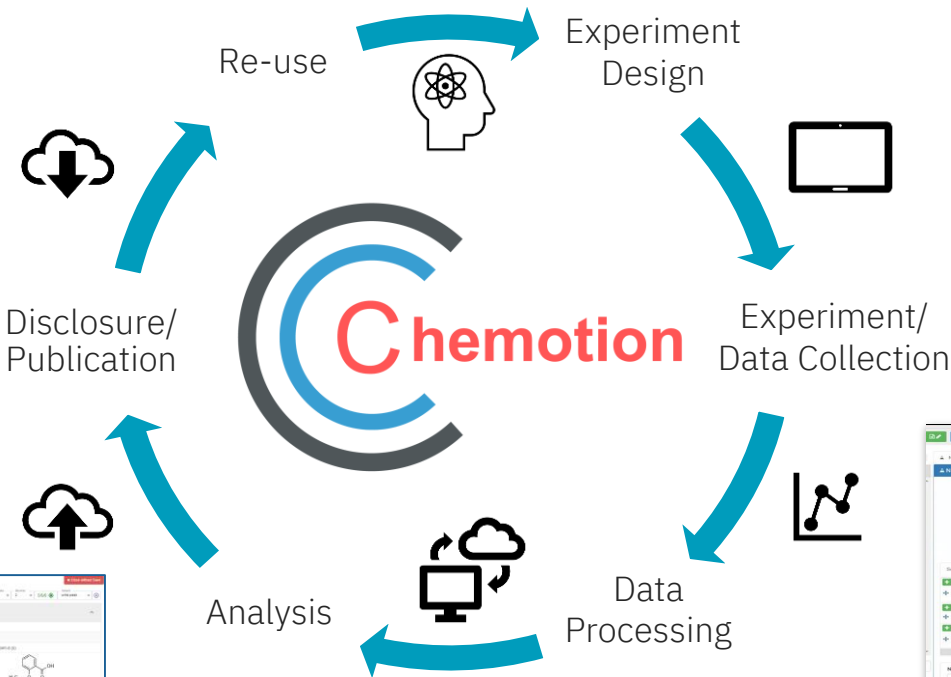
Federated
Repositories

Chemotion – ELN & Repository



Chemotion-Repository Publications Newsroom 1 How To 0

ID	Embeugo	Autor	Análisis	X-Total
CRS-1953		Johanne Klein	Análisis 8	X-Total
CRS-1950		Christoph Zippel	Análisis 4	X-Total
CRS-1787		Christoph Zippel	Análisis 4	X-Total



Experiment Design Interface

Name: [] Status: **Successful** Temperature: 100

Start: 22/09/2021 09:04:11 Stop: 22/09/2021 10:00:00 Duration: 2 hours 55 min 56 s Input Duration: []

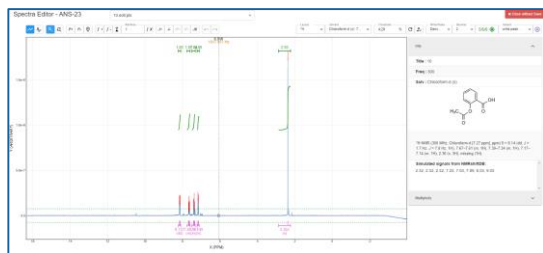
Type (Name Reaction Ontology): [] Role: []

Description: []

Purification: []

Purification Scheme	Label	Vol	Vol ratio
+ Water	Water	38.8	1.0
+ 1,4-Dioxane	1,4-Dioxane	38.8	1.0

Additional information for publication and purification details: []



Experiment/Data Collection Interface

Name: [] Status: [] Temperature: []

Reaction:

Reaction	Yield	Amount	Time	Temp	Status	Exp.
1. 1st Attempt	0.00	0.00	0.00	0.0	Success	1.00
2. 2nd Attempt	0.00	0.00	0.00	0.0	Success	1.00
3. 3rd Attempt	0.00	0.00	0.00	0.0	Success	1.00

Name: [] Status: [] Temperature: []

Description: []

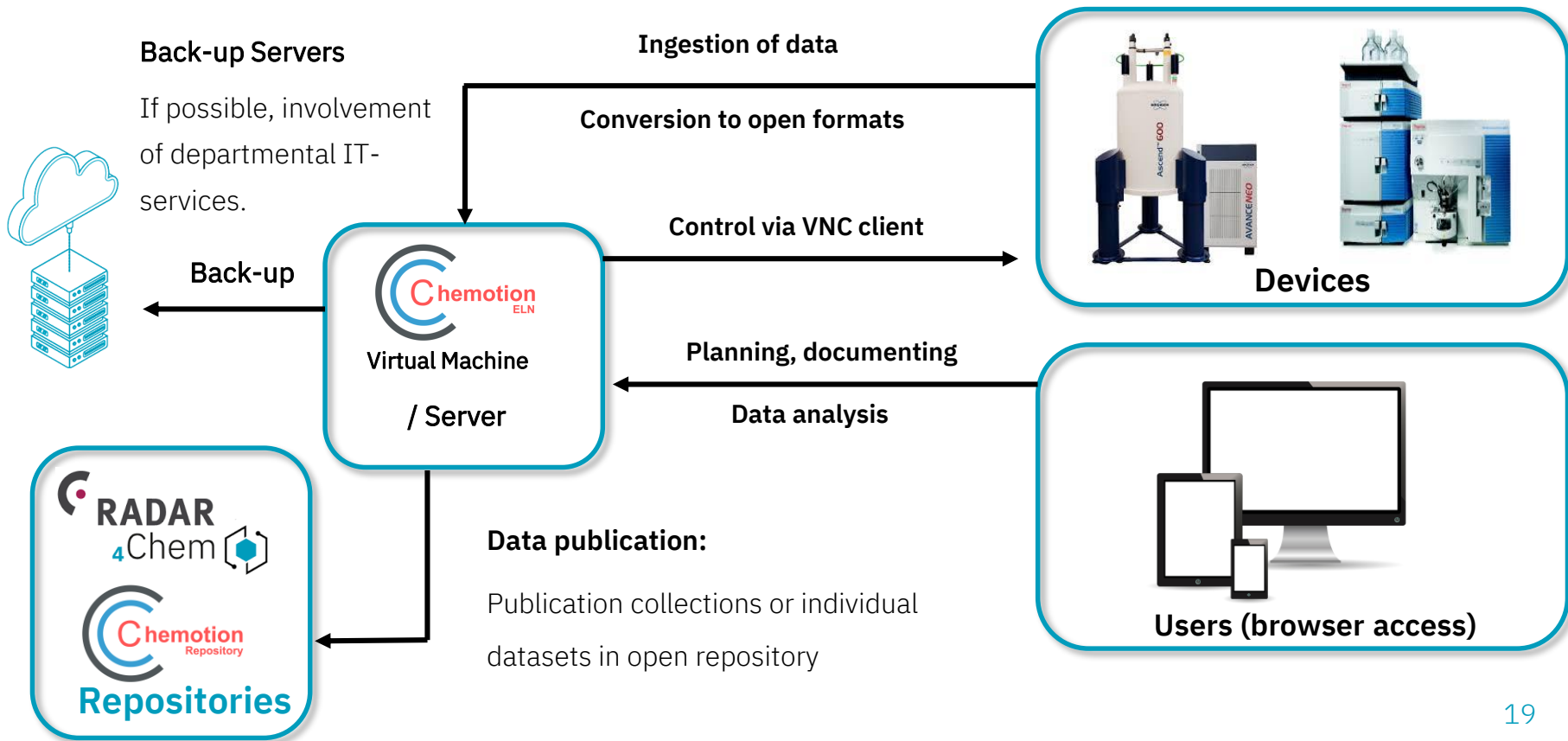
Chemotion – Quick Facts



- 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 - Setup



Chemotion - Basic view



Chemotion - All - IUPAC, InChI, SMILES, RInI

128(0) 1751(0) 3(0) 11(0)

From To

NJ-R1591

1.0

NJ-R1566

1.0

NJ-R1590

1.0

NJ-R1578

NJ-R1565

1.0

NJ-R1577

NJ-R1589

1 2 3 4 5 ...

Show 15

NJ-R1591

1.0

Reaction scheme showing the synthesis of 2-bromoquinoxaline from 1H-quinoxalin-2-one and tetrabutylammonium bromide (TBAH) in toluene at 100 °C for 2.5 hours, yielding 77%.

Scheme Properties Literature Analyses

Starting materials

Ref	L/ST/RAmount	Conc	Equiv
NJ-2940 1H-quinoxalin-2-one	100.0 mg 0.00 ml 0.6842 mmol 6.842 mmol 1.000		

Reactants

Reagents	L/ST/RAmount	Conc	Equiv
tetrabutylazanium, bro...	220.6 mg 0.00 ml 0.6842 mmol 6.842 mmol 1.000		
O10P4	194.3 mg 0.00 ml 0.6842 mmol 6.842 mmol 1.000		

Products

L/ST/RAmount	Conc	Yield
NJ-2943 NJ-R1591-... 2-bromoquinoxaline	110.0 mg 0.00 ml 0.5262 mmol 5.262 mmol 77%	

Solvents Conditions

Name: Name... Status: Successful Temperature: 100 °C

Start: DD/MM/YYYY hh:mm:ss Stop: DD/MM/YYYY hh:mm:ss Duration: 2.5 /hour(s)

Type (Name Reaction Ontology) Role

Chemotion - Generic Elements



- For non-synthetic workflows
- Create your own workflows

Lab  Motion

Template [Preview](#)

Template of Element [catch] ver: e75427f4-4ccf-4a0b-ba57-c9da9877229 draft: dc3a99a7-9a95-4a99-92c2-ca22c19be95

Layers Add new layer +

Reaction table for catalyst testing of type II table Columns per Row: 1 Fields: 1 🔍 ✎ 🗑️ Input new field name + 🔍

1 components 🔍 ⬆️ ⬇️ ⬆️ 🗑️

Characterization charc Columns per Row: 4 Fields: 3 🔍 ✎ 🗑️ Input new field name + 🔍

1 type_char 🔍 ⬆️ ⬇️ ⬆️ 🗑️

2 type_char2 🔍 ⬆️ ⬇️ ⬆️ 🗑️

3 type_char3 🔍 ⬆️ ⬇️ ⬆️ 🗑️

Gas characterization gas Columns per Row: 1 Fields: 1 🔍 ✎ 🗑️ Input new field name + 🔍

1 analyses 🔍 ⬆️ ⬇️ ⬆️ 🗑️

Type of experiment type Columns per Row: 1 Fields: 1 🔍 ✎ 🗑️ Input new field name + 🔍

1 setting 🔍 ⬆️ ⬇️ ⬆️ 🗑️

Reaction table for catalyst testing of type II

Components +

Role of sample	Sample	Short label	Name	Ext. Label	Amount	Volume	Equivalents/loading
(No data)							

Characterization

Catalyst characterization Gas phase characterization Others

Gas characterization

Gas analysis Drop File, or Click to Select.

Type of experiment

Setting Select...

Batch experiment - device and setting

Device - Used reactor 🗑️ Temperature °C Time

Stir rate Observation Pressure alm



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

The screenshot displays the Chemotion ELN interface for analyzing 1-octylindole. The left sidebar shows a collection of samples, including 1-octylindole (SG-V0949) and 1H-indole-5-carbonitrile (X0061). The main view shows the chemical structure of 1-octylindole and its NMR spectra. The analysis panel on the right provides detailed information for 1H NMR, 13C NMR, and IR spectra, including peak lists and integration values.

The screenshot displays the Chemotion ELN interface for analyzing N-(2-aminyl-7-(difluoromethyl)indolizin-3-yl)-2-phenylacetamide. The left sidebar shows a collection of samples, including 8-bromo-2,6-dimethyl-1-oxopyridin-1-ium (C17H18NO) and N-(2-aminyl-7-(difluoromethyl)indolizin-3-yl)-2-phenylacetamide (SG-V0949). The main view shows the chemical structure of the compound and its NMR spectra. The analysis panel on the right provides detailed information for 1H NMR, 13C NMR, and IR spectra, including peak lists and integration values.

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/>




<https://t1p.de/b13zw>

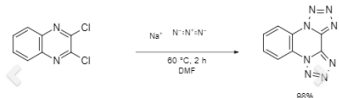
Repository for samples, reactions and related research data

research data repository




this repository is part of the strategy of



Published 5 days ago by Laura Holzhauser



99%

	3474 published 574 under review 1463 under embargo
	1683 published 608 under review 1445 under embargo
	12753 published Top 3: 5066 NMR 2688 IR 2430 Mass

Data in the Chemotion Repository



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

Chemotion-Repository My DB Data publications Molecule Archive Review Embargoed Publications Newsroom How-To LabIMotion John Jolliffe

Search: [Q]

ID	Embargo	Author	Published on	Analyses	X-Vial
CRS-33186		Lisa Schmidt	2023-08-02	8	[Icon]
$C_{24}H_{25}Si_4$ trimethyl-[2-[4-[tris[4-(2-trimethylsilylethynyl)phenyl]methyl]phenyl]ethynyl]silane					
CRS-32980		Lisa Schmidt	2023-08-02	7	[Icon]
$C_{22}H_3BrClN$ 4-(11-bromo-5-tricyclo[8.2.2.2.4.7]hexadeca-1(12),4,6,10,13,15-hexaenyl)-1-methylpyridin-1-ium, chloride					
CRS-33144		XUJUN QIU	2023-07-31	4	-
$C_{13}H_{13}NO_2$ [6-(cyclopropylmethoxy)-1H-indol-2-yl]methanol					
CRS-34611	NPK_2023-06-05	Niklas Krappel	2023-07-31	8	[Icon]
$C_{23}H_{22}BrNO_4$ (4-methoxyphenyl)methyl 6-bromo-1-(4-methoxyphenyl)methylindole-4-carboxylate					
CRS-34730	NPK_2023-06-05	Niklas Krappel	2023-07-31	9	[Icon]

1 2 3 4 5 ... Show 10

View

IUPAC Name: 4-(11-bromo-5-tricyclo[8.2.2.2.4.7]hexadeca-1(12),4,6,10,13,15-hexaenyl)-1-methylpyridin-1-ium, chloride ($C_{22}H_3BrClN$)

Canonical SMILES: C[n+](c1ccc(cc1)c1cc2ccc1CCc1ccc(CC2)(c1)Br[Cl-]

InChI: InChI=1S/C22H3BrClN.ClH/c1-24-12-10-19(11-13-24)21-14-16-2-6-18(21)7-3-17-5-9-20(8-4-16)22(23)15-17/h2,5-6,9-15H-3,4,7-8H2,1H3,1Hq+1,p-1

InChIKey: HAUKGWOQLXZEJP-UHFFFAOYSA-M

Exact Mass: 413.054589 g·mol⁻¹

Crosslinks: [Icon] 1st

Sample Published on 2023-07-31

Contributor: XUJUN QIU

1. IOAK Bräse, Karlsruhe Institute of Technology, Germany

Authors: XUJUN QIU¹ - Stefan Bräse^{2,3}

1. IOAK Bräse, Karlsruhe Institute of Technology, Germany

2. Institute of Organic Chemistry, Karlsruhe Institute of Technology, Germany

3. Institute of Biological and Chemical Systems, Karlsruhe Institute of Technology, Germany

Sample type: Consists of molecule with defined structure

Sample DOI: 10.14272/HALUKGWOQLXZEJP-UHFFFAOYSA-M.1 [Icon] [JSONLD]

Sample ID: CRS-33144 [Icon]

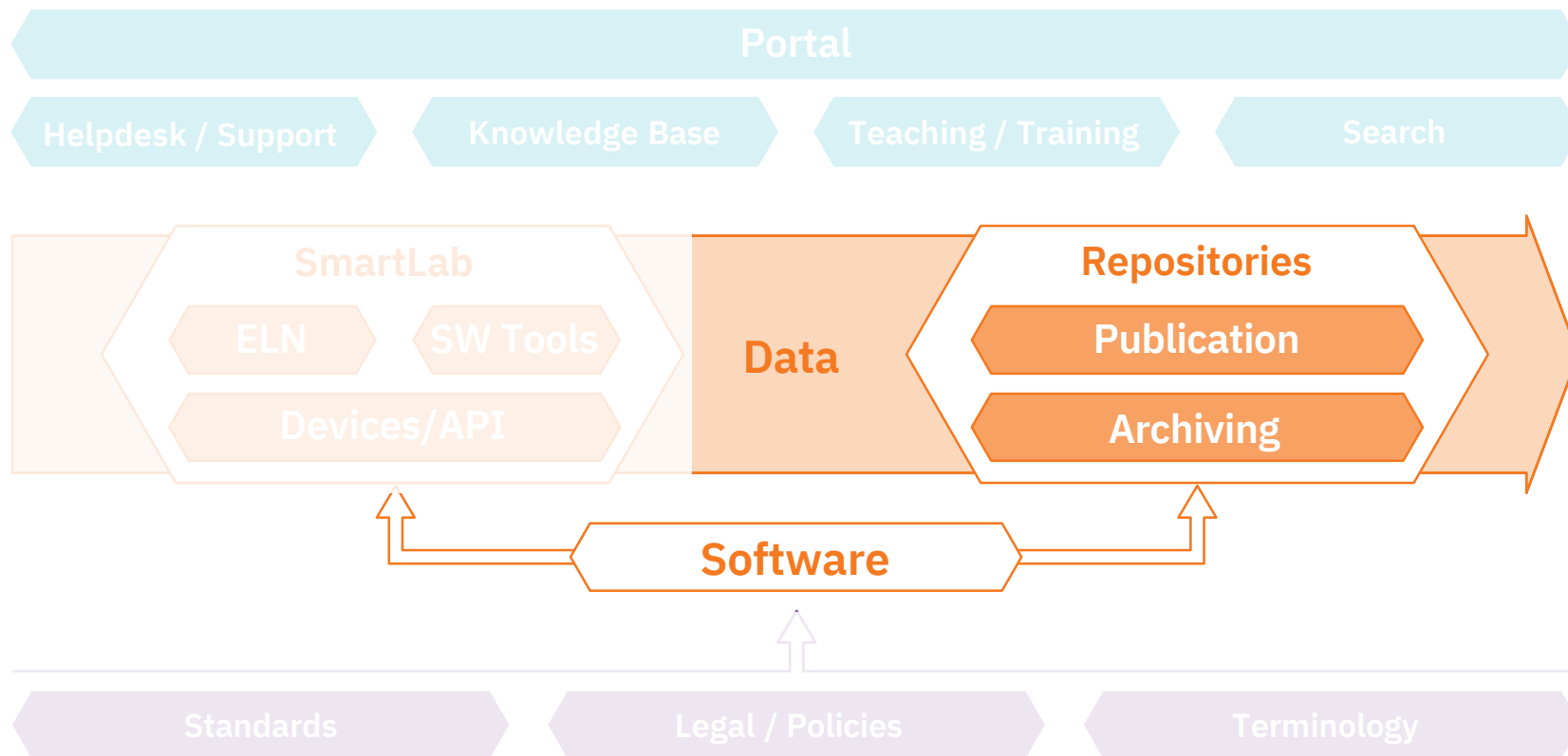
Relations of this sample: Is Product of a reaction [Icon], has analytical data [Icon]

Reference in the Literature:

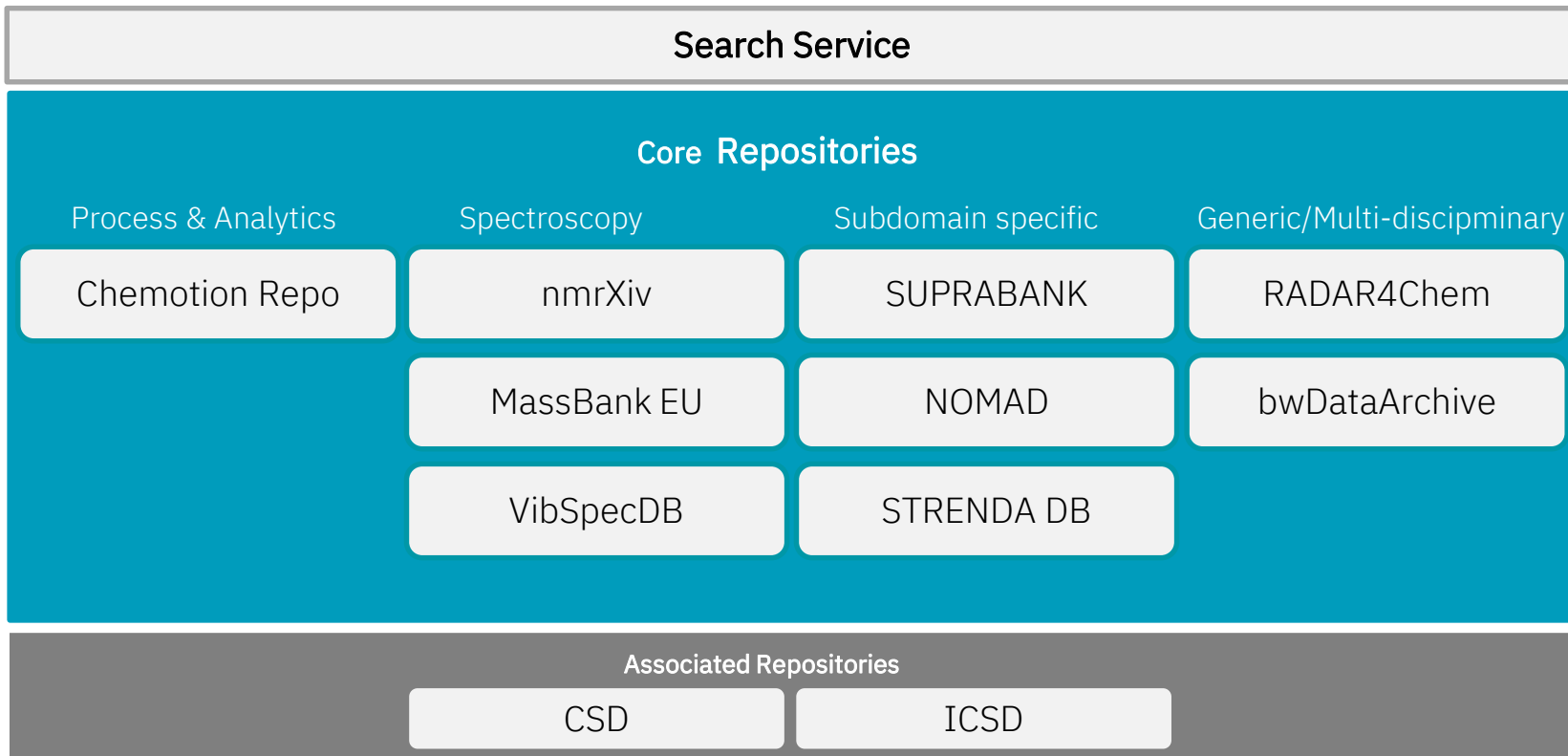
Physical Properties:
Melting point: 221.6 °C
Boiling point:

1H NMR, 13C NMR, IR, MS

ELNs & Repositories



Federation of Repositories



Knowledge Base



Portal

Helpdesk / Support

Knowledge Base

Teaching / Training

Search

SmartLab

ELN

SW Tools

Devices/API

Data

Repositories

Publication

Archiving

Software

Standards

Legal / Policies

Terminology

NFDI4Chem Knowledge Base



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

NFDI4Chem Knowledge Base

A place for all knowledge regarding Research Data Management (RDM) in Chemistry

Get started

Domains Roles Handling Data Electronic Lab Notebooks Data Publication

Funded by DFG Deutsche Forschungsgemeinschaft German Research Foundation

NFDI4Chem is funded by DFG Project Number 441958208

Community: LinkedIn, Twitter, GitHub

Resources: NFDI4Chem Website, NFDI4Chem FAQ, NFDI4Chem Helpdesk, NFDI4Chem Terminology Service, NFDI4Chem Search Service, NFDI4Chem Knowledge Base Git Hub Repository

Legal information: About, Legal Notice, Privacy

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<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

Coordination
chemistry



Digital Documentation in the ELN



Processing of the synthesis of Ferrocene in the Chemotion ELN

The screenshot displays the Chemotion ELN interface for the synthesis of ferrocene. It includes a reaction scheme showing the reaction of cyclopentadienyl sodium with iron(II) chloride, a 1H NMR spectrum with a peak at 4.25 ppm, and a data entry form with the following details:

- Name:** Ferrocene
- Type (Name Reaction Ontology):** Normal
- Description:** The reaction has been conducted in dry glass vial. Solvent cyclopentadiene (1.6 g, 1.5 mmol, eq) was added in small portions. Afterwards, it added to the mixture to quench the remaining unreacted ferrocene. The mixture was filtered through diatomaceous earth and the filter cake was dried at 100 °C to yield ferrocene (7.68 g, 41.3 mmol, 64% yield).
- Purification:** Sublimation
- Purification Solvents:** Default solvents, Pentane
- 1H NMR:** 1H NMR (43 MHz, Chloroform-d [7.27 ppm], ppm) δ = 4.25 (s, 10H)

Coordination chemistry



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

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

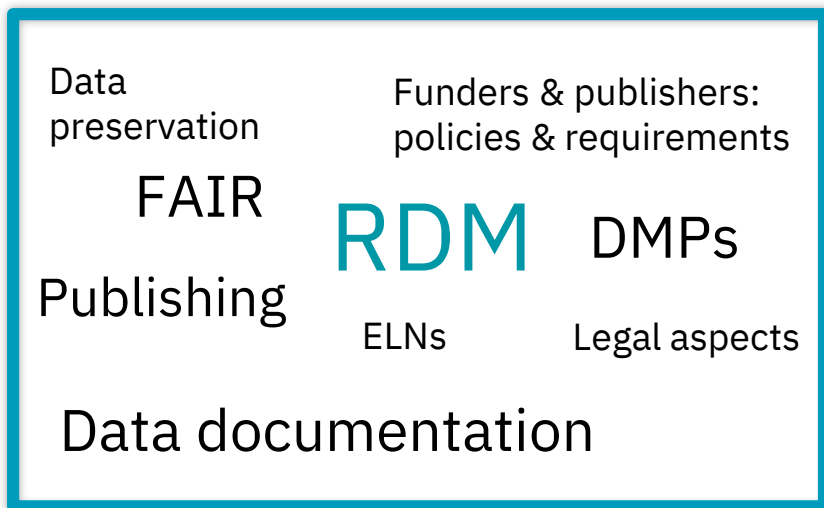
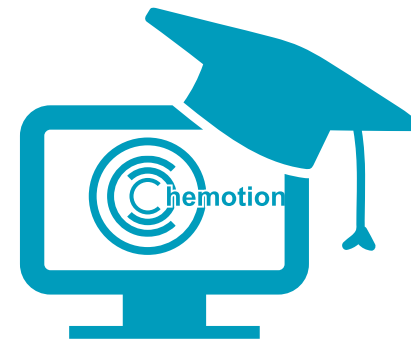
Chem. Methods **2022**,
2 (10), e202200026.



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**



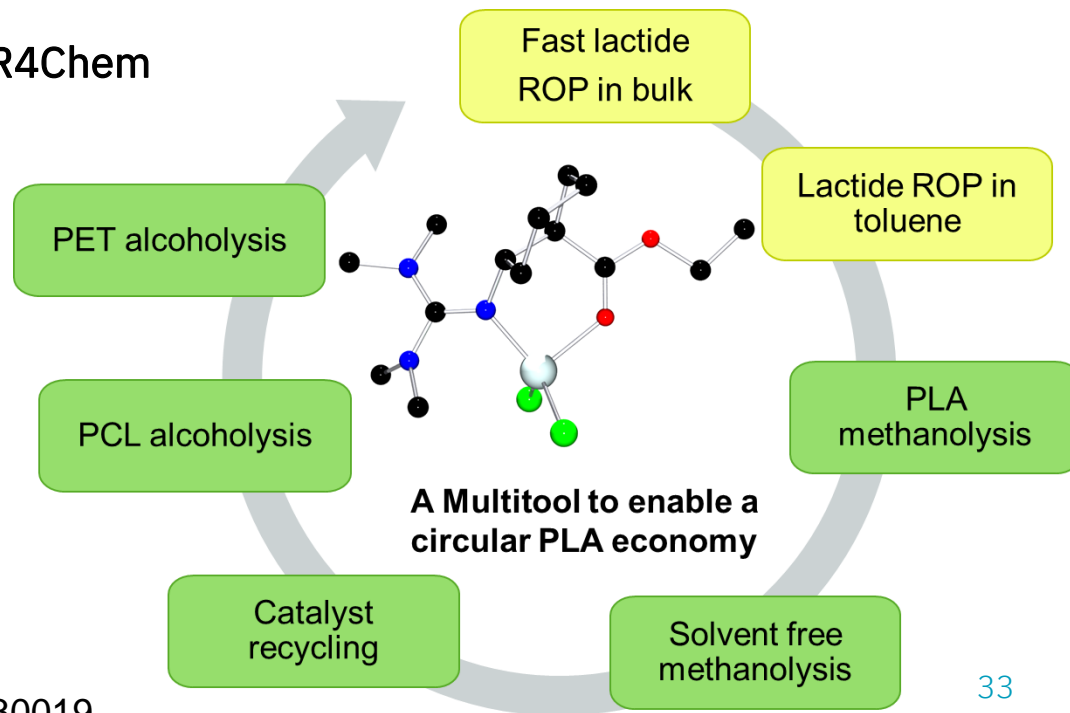
<https://t1p.de/aw72j>

Best Practices



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

- **Disciplinary examples and interdisciplinary examples**



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twitter.com/Nfdi4Chem

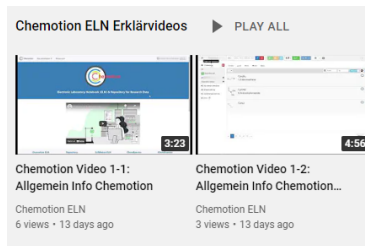
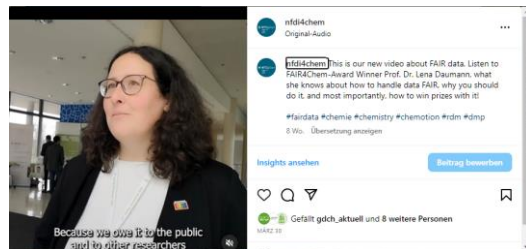


[instagram.com/nfdi4chem/](https://www.instagram.com/nfdi4chem/)



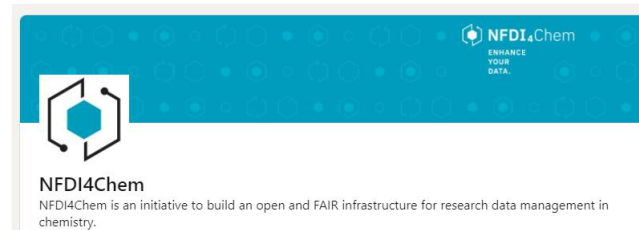
[youtube.com/@nfdi4chem251](https://www.youtube.com/@nfdi4chem251)

Homepage: nfdi4chem.de



NFDI4Chem
@NFDI4Chem

Great to see everyone in person at our [#NFDI4chem](#) meeting in [#hannover](#). Thank you to everyone who participated - especially to our advisory board members. The future is bright for [#FAIR #data in #chemistry](#). [@GDCh_aktuell](#) [@JungChemiker](#) [@NFDI_de](#) [@NFDI4Cat](#) Credit: TIB/C. Bierwagen



NFDI4Chem

NFDI4Chem is an initiative to build an open and FAIR infrastructure for research data management in chemistry.

Welcome

Dear reader,

Just in time for Christmas, we are delighted to present our first NFDI4Chem newsletter. With the official start of the NFDI4Chem project on 1 October 2020, the consortium is gaining momentum and getting on track. In this first issue we report on the virtual kick-off meeting in October, our first Data Pledge, best practises for using data repositories, latest publications from the consortium, the upcoming joint webinar on ontologies and we announce our "Stammtisch" on Electronic Lab Notebooks.

With the next issue, we will start to introduce the six task areas of NFDI4Chem and the people behind them in more detail. Look forward to comprehensive reports of key topics of NFDI4Chem and NFDI. We will continue to inform you about upcoming events and report on past ones in detail. We will be excited to welcome you at one of our community workshops. Of course, we also keep you informed about what is happening in the NFDI and our cooperation with other consortia. Let us know if you are interested in further topics we should cover.

Enjoy the read!

Merry Christmas and a good start into the year 2021.



Your NFDI4Chem Team

Get to know the consortium!



Thank you for Listening! – Any Questions?



Composition of the consortium



FRITZ-HABER-INSTITUT
 MAX-PLANCK-GESELLSCHAFT

BAM
 Bundesanstalt für
 Materialforschung
 und -prüfung

D B G
 Deutsche Bunsen-Gesellschaft
 für physikalische Chemie e.V.

CIC

RWTH AACHEN
 UNIVERSITY

IPB Leibniz-Institut für
 Pflanzenbiochemie

Technische Universität Braunschweig

GDCh
 GESELLSCHAFT
 DEUTSCHER CHEMIKER

Universität Stuttgart

BEILSTEIN INSTITUT

tu technische universität
 dortmund

UNIVERSITÄT GREIFSWALD
 Wissen lockt. Seit 1456

DPhG
 Deutsche Pharmazeutische Gesellschaft e.V.

JGU
 JOHANNES GUTENBERG
 UNIVERSITÄT MAINZ

KIT
 Karlsruher Institut für Technologie

Chemotion LN

FIZ Karlsruhe
 Leibniz-Institut für Informationsinfrastruktur

Leibniz ipht
 LEIBNIZ-INSTITUT für
 PHOTONISCHE TECHNOLOGIEN

LMU

TECHNISCHE UNIVERSITÄT DRESDEN

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SAVE THE DATE:



2. Workshop Ontologies4Chem

11. - 12.10.2023

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