

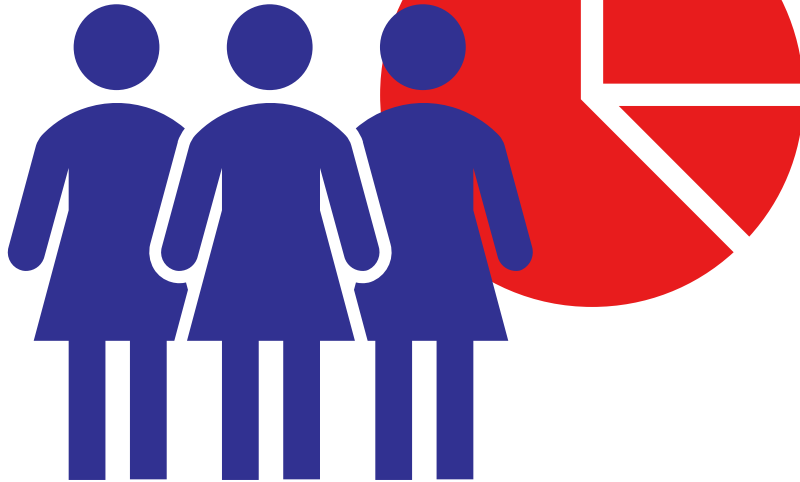
Einführung in das elektronische Laborbuch Chemotion ELN

Dr. Benjamin Golub & Anna-Karina Renziehausen



- Was ist ein ELN?
- Exkurs: NFDI und NFDI4Chem
- Chemotion ELN & LabIMotion
- Chemotion ELN - Live Demo

wooclap



LabIMotion

Was ist ein ELN?

Einfaches System: Leere Seite (Blank Sheet)

- Texteingabe
- Notizen hinzufügen
- Dateien hinzufügen (z. B. Bilder, Tabellen)
- Teilen von Inhalten
- Suchfunktionen

z. B. Evernote, Google Drive, Dropbox, MS Sharepoint

Elektronisches Laborbuch (ELB, ELN)

- + Strukturierte Metadaten in menschen- und maschinenlesbaren Formaten
- + Verknüpfung von Daten und Dokumentation
- + Disziplinspezifische Funktionen/Editoren
- + Rechtemanagement
- + Audit Trails
- + API (Application Programming Interface)

z. B. Labfolder, eLabFTW, Rspace, Labguru

Labor-Informations- Management Systeme (LIMS)

- + Probenmanagement
- + Instrument/Geräteintegration
- + Elektronische Unterschrift
- + Berichtswesen
- + Statistik

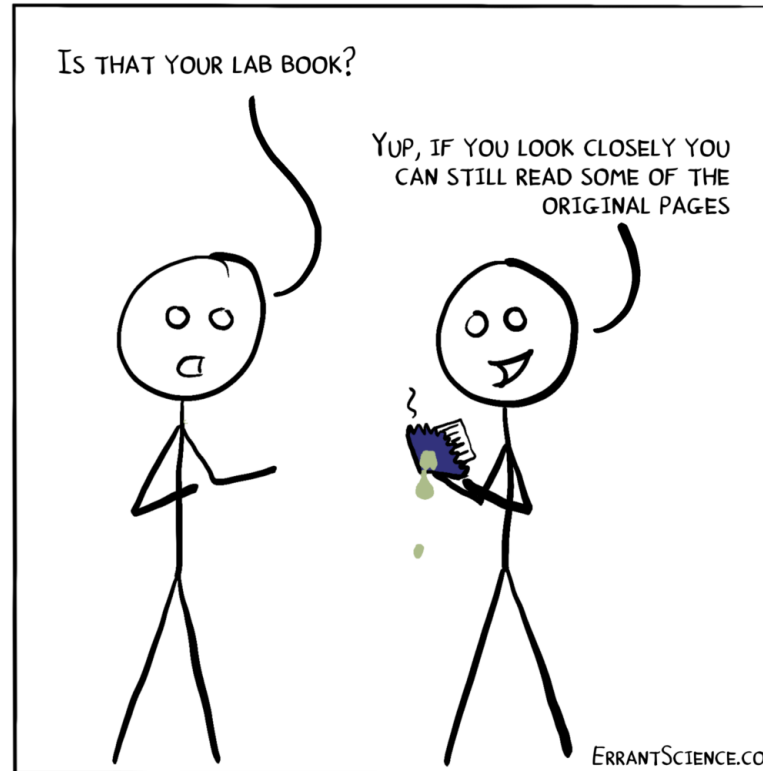
z. B. Benchling, Starlims, Limesophy

Datenverlust vermeiden

- Verlinken von Experimentbeschreibung und Dokumentation mit gesammelten Daten (analog und digital)
- Sicherer Datenspeicher und Back-up

Standardisiere Dokumentation

- Strukturierte und standardisierte Sammlung von Metadaten
- Erzeugung von interoperablen (Meta)Daten



CC-BY-NC – ErrantScience (https://errantscience.com/wp-content/uploads/200415-lab_books-1024x1024.png)

Wissensmanagement

- Daten sind auffindbar
- Daten sind zugänglich
- Daten sind verfügbar, auch nach einem Personalwechsel

Veröffentlichung

- Datenbereitstellung für die Veröffentlichung von Forschungsdaten
- Einfacher Transfer von Daten in Repositorien

Eine vielfältige Auswahl



... und viele mehr



Eine vielfältige Auswahl

- | | | | |
|----------------------------|--------------------|------------------------|------------------------------|
| ▶ AI4Green | ▶ eJournal | ▶ LabFolder | ▶ Open Inventory |
| ▶ ACAS | ▶ eLabFTW | ▶ Labguru ELN | ▶ openBIS |
| ▶ Active LN | ▶ eLabJournal | ▶ Labii | ▶ OpenText ELN |
| ▶ AgiLab ELN | ▶ eLabNotes | ▶ LabKey ELN | ▶ PatentSafe ELN |
| ▶ Agilent SLIMS | ▶ EmsoChemLab | ▶ LabLog | ▶ quattro/LJ |
| ▶ Alchemy ELN | ▶ Espresso ELN | ▶ LabsForm | ▶ RedFox |
| ▶ Arxspan ELN | ▶ eStudy | ▶ LabSpace | ▶ Rspace |
| ▶ Benchling ELN | ▶ eSystems | ▶ LabStep | ▶ SampleDB |
| ▶ BioChemLab Solutions ELN | ▶ E-WorkBook | ▶ LabTrack ELN | ▶ Sapio Seamless ELN |
| ▶ BioRails | ▶ Formulator | ▶ LabTrove | ▶ SciCord ELN/LIMS |
| ▶ Biovia Notebook | ▶ Gene Inspector | ▶ LabVantage | ▶ Sciformation ELN |
| ▶ Bookitlab | ▶ GenoFAB | ▶ LabWare ELN | ▶ Sciligence ELN |
| ▶ CBIS E-Notebook | ▶ GOLims | ▶ Laby | ▶ SciNote |
| ▶ CDD Vault ELN | ▶ Herbie | ▶ Limsophy LIMS | ▶ Signals ELN |
| ▶ CERF 5.0 | ▶ InELN | ▶ LogBook | ▶ Stackwave ELN |
| ▶ ChemCart ELN | ▶ iLES Platform | ▶ Logilab | ▶ STARLIMS ELN |
| ▶ Chemia | ▶ iQ | ▶ LOGS-ELN | ▶ Studylog |
| ▶ Chemotion | ▶ Kadi4Mat | ▶ Mbook | ▶ Sun Bio ELN |
| ▶ Colabra ELN | ▶ LabArchives | ▶ MyLabBook | ▶ Thermo Scientific Core ELN |
| ▶ CompuDrug ELN | ▶ LabCloud | ▶ NotebookMaker | ▶ Waters NuGenesis |
| ▶ Dotmatics ELN | ▶ LabCollector ELN | ▶ Online ELN Worksheet | |

- Ein Tool das bei der Wahl des passenden ELNs helfen kann
- Zurzeit mit 43 ELN-Einträgen



The ELN Finder helps you to search and select a suitable Electronic Lab Notebook (ELN) for your purposes.

- More than 40 filter criteria available.
- Filter criteria clearly divided into categories.
- Result list of the identified ELN tools displayed in an overview.
- Brief descriptions of the individual tools included.

DEMO

Was sind die Unterschiede?

Generische ELNs

Disziplin-spezifische ELNs



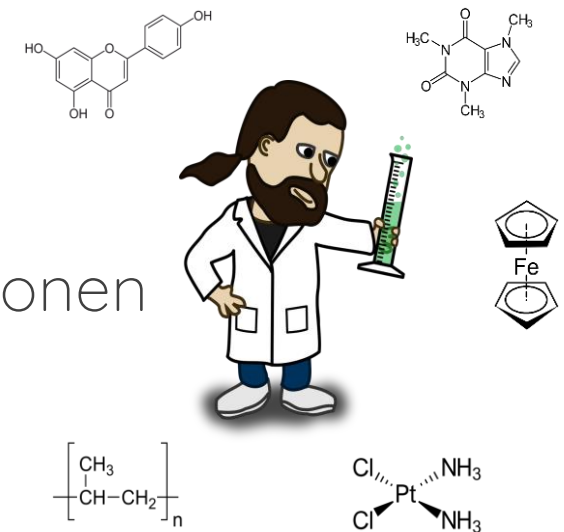
20.08.2024 – Einführung in das elektronische
Laborbuch eLabFTW, 11:00 – 12:30 Uhr

[Informationen & Anmeldung](#)



Lab  **Motion**

- Entwickelt am Karlsruher Institut für Technologie, Weiterentwicklungen im Rahmen von NFDI4Chem
- <https://www.chemotion.net/docs/elc>
- ELN für Chemie (und Chemie-nahe Disziplinen)
- Feature:
 - Open Source, [Chemotion on GitHub](#)
 - Browser-basiert
 - Zeichnen von chemischen Strukturen
 - Generieren, beschreiben und dokumentieren von Reaktionen
 - Analyse von Spektren & Charakterisierung von Proben
 - Nutzermanagement: Zugriffsrechte, Teilen von Inhalten
 - Generische Erweiterung mit [LabIMotion](#)



Exkurs:
Nationale Forschungsdateninfrastruktur
&
NFDI4Chem



NFDI₄Chem

ENHANCE
YOUR
DATA.

- Nationale Forschungsdateninfrastruktur
 - Förderung von Wissenschaft und Forschung durch eine nationale Forschungsdateninfrastruktur
 - Entwicklung eines übergreifenden FDM
 - Steigerung der Effizienz der Wissenschaft
- Bund & Länder gefördert bis einschließlich 2028
- Bis 90 Millionen Euro
- Fachbereiche werden durch 26 Konsortien vereint
- Webseite der NFDI -> <https://www.nfdi.de/>



Nationale
Forschungsdaten
Infrastruktur

Die Konsortien der NFDI

Geförderte Konsortien (Runde 1)



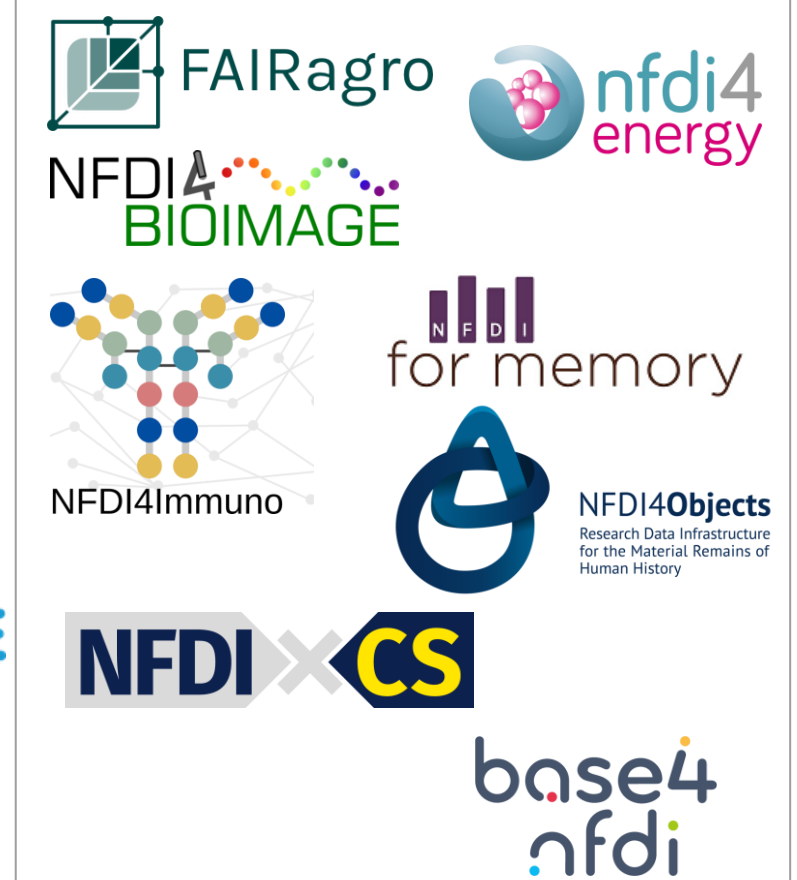
(22 Anträge, 9 akzeptiert, Oktober 2020)

Geförderte Konsortien (Runde 2)



(17 Anträge, 10 akzeptiert, Oktober 2021)

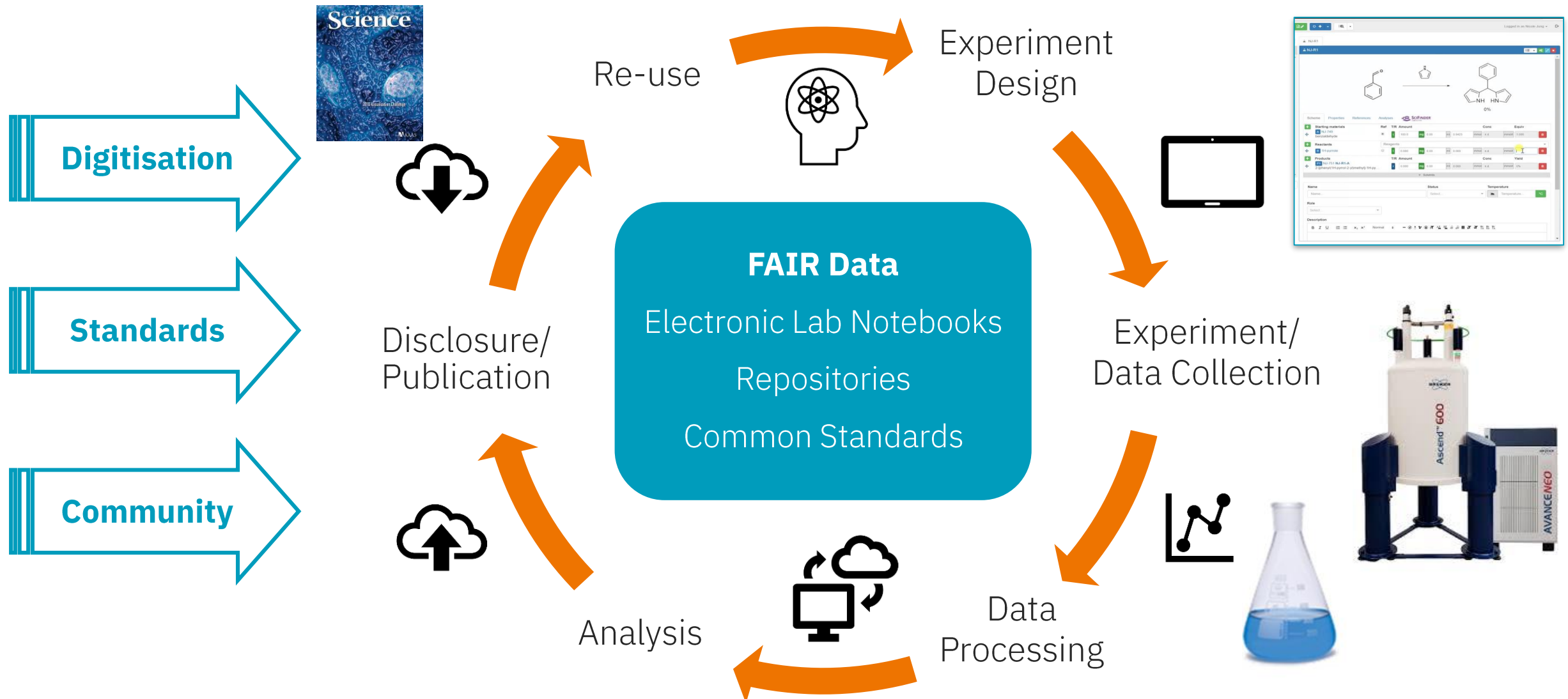
Geförderte Konsortien (Runde 3)



(16 Anträge, 8 akzeptiert, November 2022)

Die Konsortien der NFDI





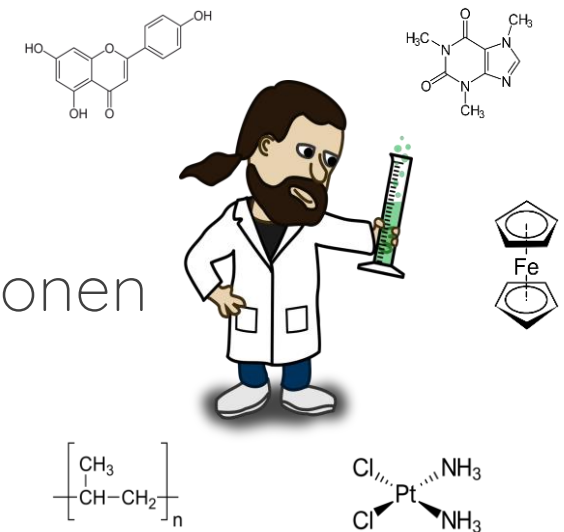
Mitglieder von NFDI4Chem



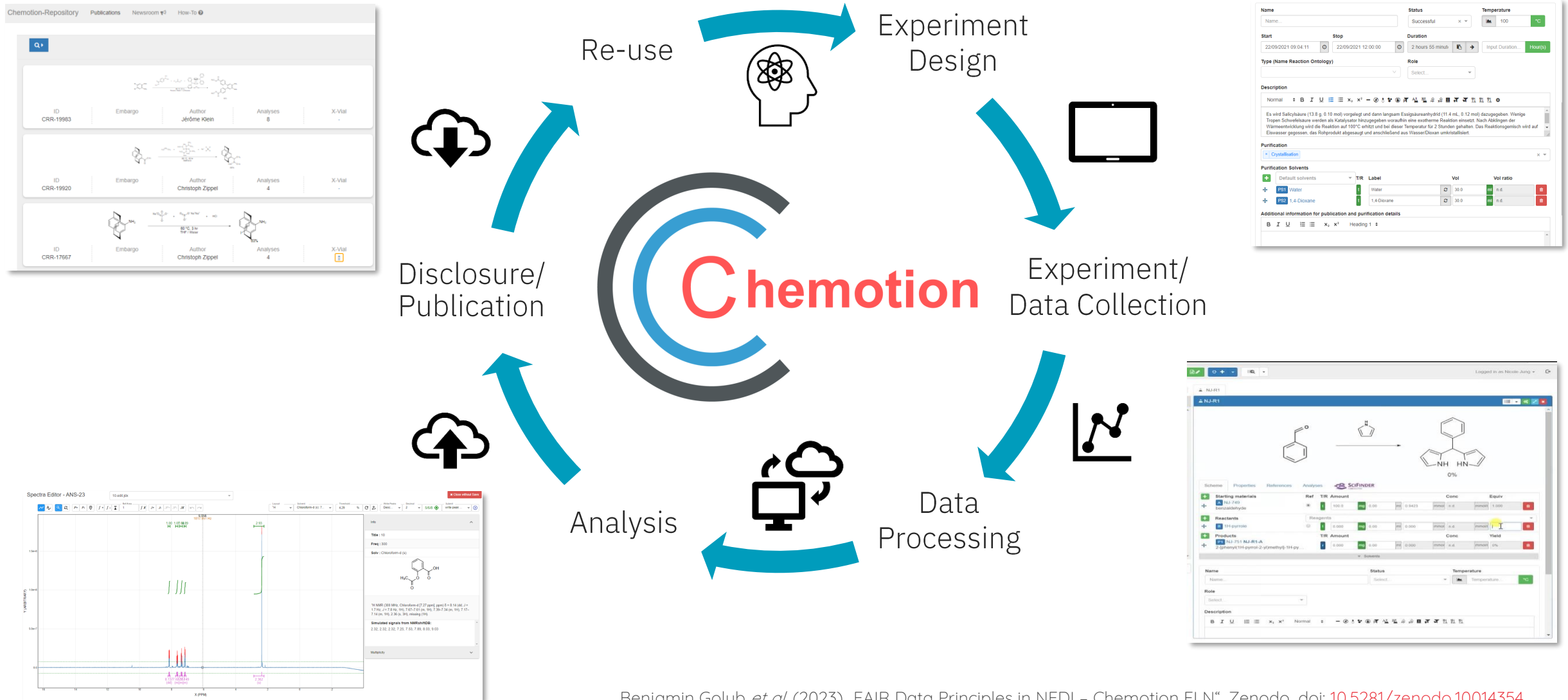
Gibt es Fragen?



- Entwickelt am Karlsruher Institut für Technologie, Weiterentwicklungen im Rahmen von NFDI4Chem
- <https://www.chemotion.net/docs/elc>
- ELN für Chemie (und Chemie-nahe Disziplinen)
- Feature:
 - Open Source, [Chemotion on GitHub](#)
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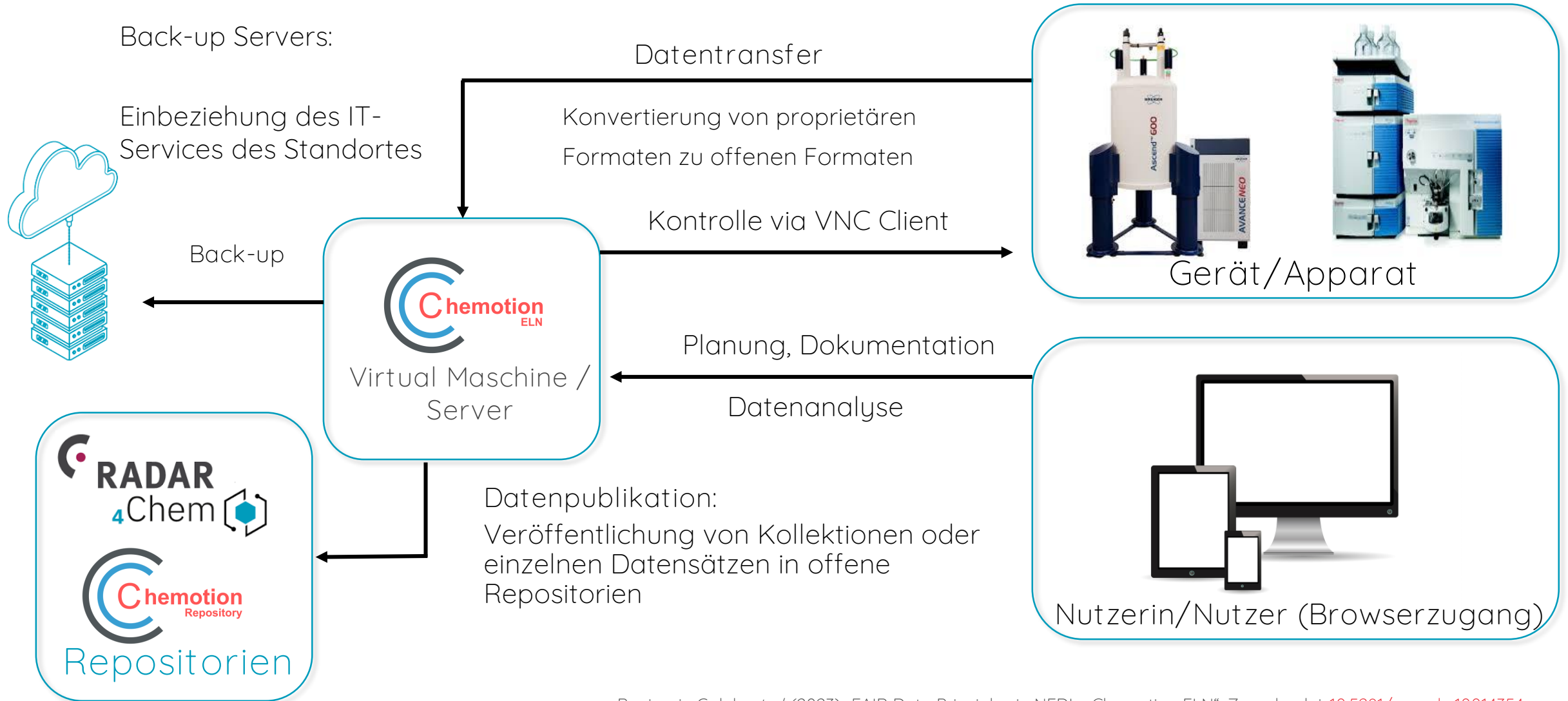


Chemotion ELN & Repositorium



Benjamin Golub *et al.* (2023) „FAIR Data Principles in NFDI – Chemotion ELN“. Zenodo, doi: [10.5281/zenodo.10014354](https://doi.org/10.5281/zenodo.10014354).

Chemotion ELN – Set-up



Collection Bar

Action Bar

Element Bar

Detail Tab

The screenshot displays the Chemotion ELN interface. On the left is the 'Collection Bar' with a list of collections including 'chemotion-repository.net', 'Test Collection Data', 'Lamella Example', 'MOF Test collection', 'SurMoF Test Collection', 'MOF examples', 'Polymers', 'Linker', 'Metall-Precursor', 'Calculation Doptants', 'MOF collection', 'Info_Exchange IFG_IBCS_IOC', 'Extracted data', 'Calculation OLED', 'Calculation TADF', 'Lamella Test Collection', 'New Collection', 'My Data', 'Joachim', and 'Fabian'. Below these are 'My shared collections', 'Shared with me', 'Synchronized with me', and an 'Inbox' with 14 items.

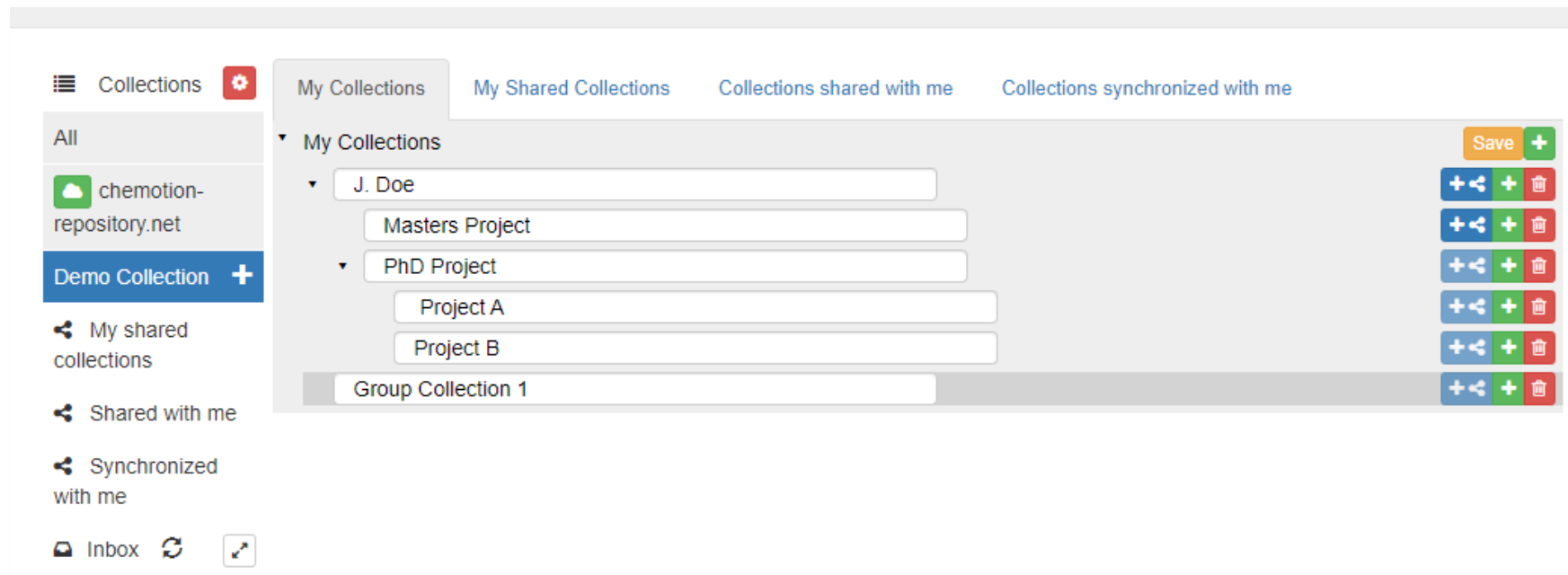
The main workspace is divided into two panes. The left pane shows a list of reactions with checkboxes and zoom controls. The right pane, titled 'Detail Tab', shows a detailed view of reaction NJ-R1591. It includes a chemical reaction scheme showing the synthesis of 2-bromoquinoline from 1H-quinoxalin-2-one, tetrabutylazanium bromide, and O10P4. The reaction conditions are 100 °C, 2.5 hr in Toluene, with a 77% yield.

Below the reaction scheme, the 'Scheme' tab is active, showing a table of starting materials, reactants, and products. The table has columns for Name, Ref, L/S/T/R/Amount, Conc, Equiv, and Yield.

Category	Name	Ref	L/S/T/R/Amount	Conc	Equiv	Yield
Starting materials	NJ-2940 1H-quinoxalin-2-one		100.0 mg	0.6842 mmol	6.842 mmol/l	1.000
Reactants	tetrabutylazanium, bro...		220.6 mg	0.6842 mmol	6.842 mmol/l	1.000
Reactants	O10P4		194.3 mg	0.6842 mmol	6.842 mmol/l	1.000
Products	NJ-2943 NJ-R1591-... 2-bromoquinoxaline		110.0 mg	0.5262 mmol	5.262 mmol/l	77%

At the bottom of the detail tab, there are fields for Name, Status (Successful), Temperature (100 °C), Start/Stop times, Duration (2.5 Hour(s)), and Role.

- Hierarchische Art der Strukturierung von Experimenten und Daten
- Standardmäßig werden Daten nur vom Ersteller gesehen
- Gemeinsame/synchronisierte Sammlungen sind innerhalb einer einzelnen Chemotion ELN-Instanz möglich



 114(0)

Samples

- Eigenschaften chemischer Verbindungen z. B. Strukturen und Kennungen

 16(0)

Reactions

- Dokumentation
- Berechnung
- Zuweisung von *Samples*
- Analyse

 3(0)

Wellplates

- 96 Wellplate
- Gestaltung und Beschreibung
- Zuweisung von *Samples*

 3(0)

Screens

- Überblick von (biologischen) Experimenten
- Mehrere *Wellplates*

 1(0)

Research Plan


- Generisch und flexible
- Texte, Tabellen, Bilder, Links zu *Reactions* und *Samples*, ...

- Samples sind zentral für *Reactions* (verlinkt als Startmaterial und Produkte) und *Wellplates* (zugewiesen zu einem Well)
- Chemische Identifier (SMILES, InChI, Molfile, CAS)
- *Decoupled sample* Modus: entkoppelt die Beschreibung einer *Sample* von der chemischen Struktur, z. B. für Mischungen oder Polymere
- Inventarfunktion

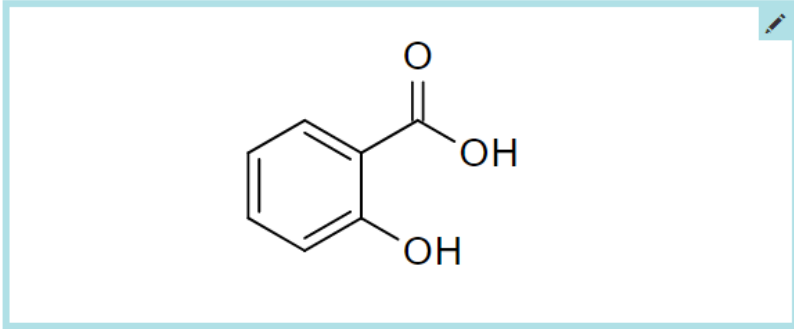
QANS-14 Salicylic acid 1-1

☐ Decoupled

C₇H₆O₃
2-hydroxybenzoic acid
138.120740 g/mol
Exact mass: 138.031694 g/mol



[Source: European Chemicals Agency \(ECHA\)](#)
[Read more about Safety Summary from PubChem](#)



Properties Analyses QC & curation Literature Polymer details Results

Molecule 2-hydroxybenzoic acid **Stereo Abs** any **Stereo Rel** any ☐ Top secret ☐ Decoupled

Name Salicylic acid **External label** SA-169 **Boiling point** °C **Melting point** °C

Amount 50.00 mg 0.0000 µl 0.0003620 mol **Density** 0.0000 g/ml **Molarity** **Purity/Concentration** 1.0000

Description

- Überblick für alle Analysen behalten
- Direktes Hinzufügen von Datensätzen (auf Server gespeichert)
- Oder verlinke den Ort des Datensatzes (z. B. Pfadlink)
- Generell können alle Datentypen hier hochgeladen werden

Scheme Properties **Analyses** References

Analysis: JDJ-R19

new
no attachment
Type:
Status:
Content:

Name
new

Status
Select...

Type (Chemical Methods Ontology)
▼

Content
Normal B I U X_2 X^2 C EA H IR UV

Description

Datasets
There are currently no Datasets.
Drop File(s) from the inbox

Hyperlinks:

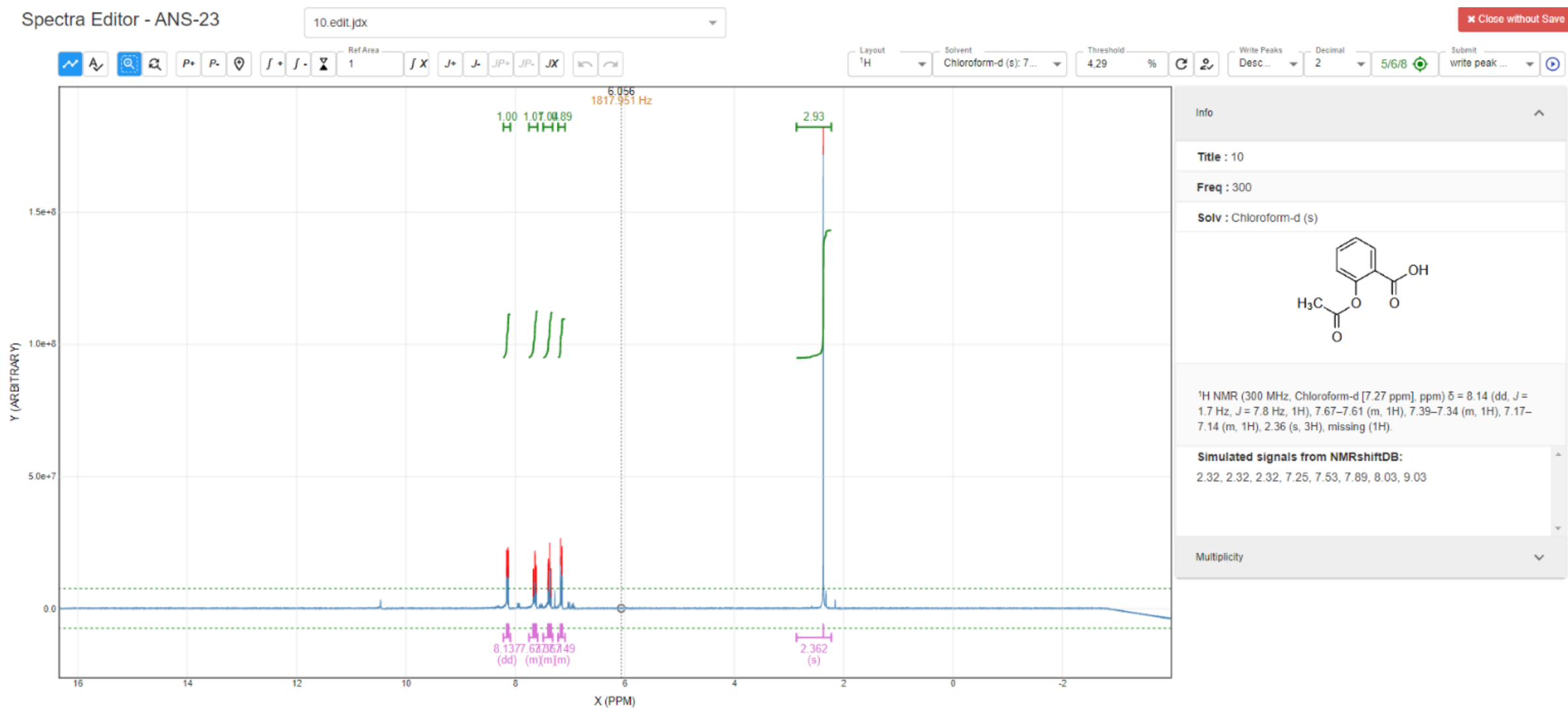
There are currently no Datasets.

Add analysis

- Für einige Datentypen, Analyse und Konvertierung in offene Datenformate möglich
- Durch Chemspectra und NMRium (open-source Tools) ist eine direkte Analyse der Daten im ELN möglich
- Geräteintegration ist möglich

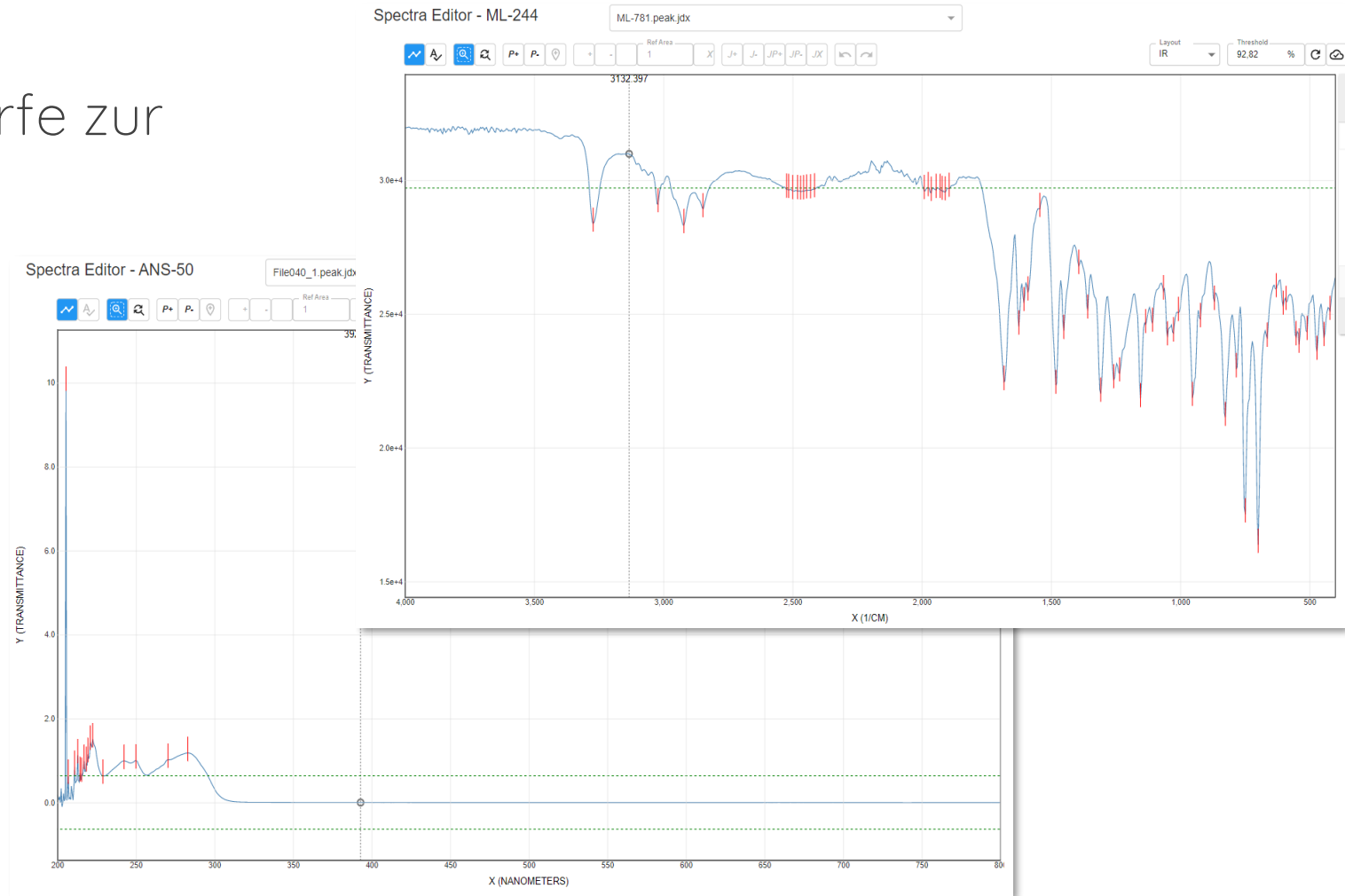
The screenshot displays the 'Analyses' tab of the FDMNDS software. It shows four analysis entries, each with a spectral plot, a title, type, status, instrument, and detailed content.

Analysis	Type	Status	Instrument	Content
1H NMR	1H nuclear magnetic resonance spectroscopy (1H NMR)	Confirmed	1/1	¹ H NMR (400 MHz, Chloroform-d [7.27 ppm], ppm) δ = 8.32 (br. s, 1H), 7.53 (dd, J = 0.9 Hz, J = 7.9 Hz, 1H), 7.41–7.39 (m, 1H), 7.28–7.24 (m, 1H), 7.18–7.10 (m, 2H), 7.06–7.00 (m, 3H), 6.73 (dd, J = 1.0 Hz, J = 7.8 Hz, 2H), 6.09 (d, J = 8.1 Hz, 1H), 4.89 (td, J = 5.9 Hz, J = 8.3 Hz, 1H), 3.73 (d, J = 0.5 Hz, 2H), 3.66 (s, 3H), 2.97 (dd, J = 2.7 Hz, J = 5.6 Hz, 2H). Impurities: This spectrum contains methylene chloride at 5.30 ppm.
13C NMR	13C nuclear magnetic resonance spectroscopy (13C NMR)	Confirmed	1/1	¹³ C NMR (100 MHz, Chloroform-d [77.0 ppm], ppm) δ = 171.8, 171.1, 136.3, 135.4, 129.0 (2C), 128.3 (2C), 127.0, 126.9, 123.6, 122.6, 120.0, 118.7, 111.3, 108.5, 52.8, 52.2, 37.6, 33.2.
IR	infrared absorption spectroscopy (IR)	Confirmed	1/1	IR (ATR, $\tilde{\nu}$) = 3417 (m), 3318 (m), 3059 (w), 3033 (w), 2955 (w), 2924 (w), 2850 (vw), 1750 (vs), 1743 (vs), 1705 (w), 1644 (vs), 1525 (vs), 1494 (w), 1456 (m), 1432 (s), 1374 (w), 1359 (w), 1348 (w), 1335 (w), 1300 (w), 1276 (m), 1263 (w), 1252 (w), 1229 (m), 1214 (vs), 1189 (m), 1168 (vs), 1120 (m), 1088 (s), 1068 (w), 1046 (w), 1027 (w), 1010 (w), 1003 (w), 981 (s), 956 (m), 932 (w), 912 (w), 877 (w), 860 (w), 843 (w), 828 (w), 782 (m), 7...
Mass	mass spectrometry (MS)	Confirmed	2/2	El (m/z, 70 eV, 140 °C): 336 (49) [M] ⁺ , 272 (14), 262 (11), 174 (15), 130 (100). HRMS (C ₂₀ H ₂₀ O ₃ N ₂): Calcd 336.1468, Found 336.1467.



ChemSpectra bietet Entwürfe zur Analyse von

- NMR (^1H , ^{13}C , ^{19}F , ^{31}P , ^{15}N , ^{29}Si)
- mit NMRium auch 2D-NMR
- IR-Spektroskopie
- UV/Vis-Spektroskopie
- Massenspektrometrie
- HPLC Chromatogramme
- Cyclovoltammetrie
-



- Dokumentation von
 - Synthesen
 - Titrationen
 - TLCs
 - ...
- Erstellung von Berichten (z. B. Supporting Informations)

ANS-R2 1-1

Name
Name...

Status
Successful

Temperature
100 °C

Start
22/09/2021 09:04:11

Stop
22/09/2021 12:00:00

Duration
2 hours 55 minuti

Type (Name Reaction Ontology)
Select...

Role
Select...

Description
Normal

Es wird Salicylsäure (13.8 g, 0.10 mol) vorgelegt und dann langsam Essigsäureanhydrid (11.4 mL, 0.12 mol) dazugegeben. Wenige Tropfen Schwefelsäure werden als Katalysator hinzugegeben woraufhin eine exotherme Reaktion einsetzt. Nach Abklingen der Wärmeentwicklung wird die Reaktion auf 100°C erhitzt und bei dieser Temperatur für 2 Stunden gehalten. Das Reaktionsgemisch wird auf Eiswasser gegossen, das Rohprodukt abgesaugt und anschließend aus Wasser/Dioxan umkristallisiert.

Purification
Crystallisation

Purification Solvents

	T/R	Label	Vol	Vol ratio
PS1 Water	t	Water	30.0 ml	n.d.
PS2 1,4-Dioxane	t	1,4-Dioxane	30.0 ml	n.d.

Additional information for publication and purification details

B I U x₂ x² Heading 1

Chemical structure: CC(=O)Oc1ccccc1C(=O)O
78%

Conc **Equiv**

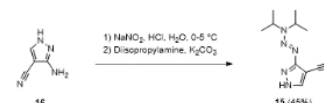
mol	n.d.	mmol/l	
mol	n.d.	mmol/l	1.200
mol	n.d.	mmol/l	1.000
mmol	n.d.	mmol/l	0.000

Conc **Yield**

mmol	n.d.	mmol/l	
mmol	n.d.	mmol/l	78%

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

5-[(E)-[di(propan-2-yl)amino]diazenyl]-1-[(H)-pyrazole-4-carbonitrile (15)



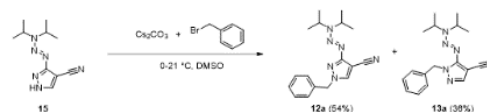
15: 5-[(E)-[di(propan-2-yl)amino]diazenyl]-1-[(H)-pyrazole-4-carbonitrile; Formula: $C_{10}H_{16}N_6$; Exact Mass: 220.1436; Smiles: CC(N(C)C)C#N=Nc1n[nH]c1C#N; InChIKey: UCPMQTTXXMXIFF-CCEZHUSRSA-N.

To a mixture of 5-amino-1H-pyrazole-4-carbonitrile (2.00 g, 19 mmol, 1.00 equiv) in 6 mL of water, conc. hydrochloric acid (6.17 mL, 74 mmol, 4.00 equiv) was added. The mixture was cooled to 0 °C and a solution of sodium nitrite (1.91 g, 28 mmol, 1.50 equiv) in 20 mL of water was added. Additional 10 mL of water were added to get a stirrable slurry. After stirring for 30 min at 0 °C, a mixture of diisopropylamine (2.43 g, 3.37 mL, 24 mmol, 1.30 equiv) and dipotassium carbonate (5.11 g, 37 mmol, 2.00 equiv) in 50 mL of water were added. The reaction mixture was stirred at 21 °C until TLC showed that all diazonium salt had disappeared. The reaction mixture was extracted with 3 × 150 mL of DCM. Some precipitate was formed between the layers which had to be filtered off (clogged the frit). The combined organic phases were washed with 3 × 60 mL of water, dried over sodium sulfate and the solvent was evaporated under reduced pressure to give the desired product. The obtained crude product was purified *via* flash-chromatography on silica gel using cyclohexane/ethyl acetate 4:1 to 2:1 to give the target compound in 45% yield (1.85 g, 8.4 mmol).

R_f = 0.08 (cyclohexane/ethyl acetate 4:1). 1H NMR (400 MHz, $CDCl_3$, ppm) δ = 9.04 (s, 1H), 7.76 (s, 1H), 5.27 (hept, J = 6.8 Hz, 1H), 4.08 (hept, J = 6.7 Hz, 1H), 1.44 (d, J = 6.6 Hz, 6H), 1.28 (d, J = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ = 158.4, 141.3, 115.4 (+, CH), 79.7, 50.8 (+, CH), 47.6 (+, CH), 23.4 (+, 2C, CH_3), 19.2 (+, 2C, CH_3); EI (m/z , 70 eV, 80 °C): 220 (100) [M]⁺, 135 (23), 134 (11), 120 (35), 109 (16), 108 (37), 100 (32), 86 (87), 84 (38), 70 (15), 69 (13), 65 (23), 58 (74), 52 (21); HRMS ($C_{10}H_{16}N_6$): Calcd 220.1436, Found 220.1438; IR (ATR, $\bar{\nu}$) = 611, 629, 643, 713, 722, 751, 771, 816, 839, 861, 880, 899, 928, 948, 1031, 1067, 1077, 1096, 1130, 1163, 1194, 1217, 1231, 1262, 1295, 1306, 1319, 1339, 1364, 1378, 1392, 1412, 1451, 1466, 1492, 1543, 1572, 1720, 1792, 2183, 2227, 2873, 2934, 2973, 3053, 3095, 3143, 3231 cm^{-1} .

Additional information on the chemical synthesis is available *via* Chemotion repository:
<https://doi.org/10.14272/reaction/SA-FUHFF-UHFFADPSC-UCPMQTTXXM-UHFFADPSC-NUHFF-NRHPV-NUHFF-ZZZ>
Additional information on the analysis of the target compound is available *via* Chemotion repository:
<https://doi.org/10.14272/UCPMQTTXXMXIFF-CCEZHUSRSA-N.1>

(E)-1-benzyl-3-(3,3-diisopropyltriaz-1-en-1-yl)-1H-pyrazole-4-carbonitrile (12a), (E)-1-benzyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-1H-pyrazole-4-carbonitrile (13a)



(E)-3-(3,3-diisopropyltriaz-1-en-1-yl)-4-carbonitrile-1H-pyrazole (15, 76.5 mg, 347 μ mol, 1.00 equiv) was dissolved in 10 mL of DMSO. Cesium carbonate (133 mg, 409 μ mol, 1.18 equiv) was added and the solution was cooled to 0 °C. Bromomethylbenzene (117 mg, 80.9 μ L, 681 μ mol, 1.96 equiv) was added and the vial was closed and slowly warmed to 21 °C. The reaction mixture was stirred at 21 °C for 48 hours. The reaction was quenched by addition of ice and was extracted with EtOAc (3 × 15 mL). The obtained organic layers were co-evaporated

with Celite(R) to give the Celite-immobilized crude product. The obtained crude product was purified *via* flash-chromatography on silica gel using cyclohexane/ethyl acetate 10:1 to 4:1, giving (E)-1-benzyl-3-(3,3-diisopropyltriaz-1-en-1-yl)-1H-pyrazole-4-carbonitrile (12a, 58.2 mg, 188 μ mol, 54% yield) as a light-orange solid and (E)-1-benzyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-1H-pyrazole-4-carbonitrile (13a, 38.7 mg, 125 μ mol, 36% yield) as a light-orange solid.

12a: (E)-1-benzyl-3-(3,3-diisopropyltriaz-1-en-1-yl)-1H-pyrazole-4-carbonitrile; Formula: $C_{17}H_{22}N_6$; Exact Mass: 310.1906; Smiles: N#Cc1c[n1N=N/C(C)C(C)C(C)C/C1cccc1; InChIKey: AONLLYWWGOIMLR-XUTLUUPISA-N

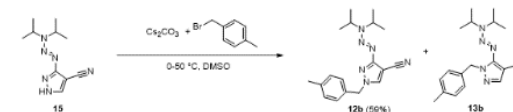
R_f = 0.23 (cyclohexane/ethyl acetate 4:1). 1H NMR (400 MHz, $CDCl_3$, ppm) δ = 7.53 (s, 1H), 7.30–7.15 (m, 5H), 5.32 (hept, J = 6.8 Hz, 1H), 5.13 (s, 2H), 3.93 (hept, J = 6.6 Hz, 1H), 1.35 (d, J = 6.6 Hz, 6H), 1.15 (d, J = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ = 162.9, 135.7 (+, CH), 134.8, 129.1 (+, 2C, CH), 128.8 (+, CH), 128.3 (+, 2C, CH), 115.3, 81.5, 56.9 (+, CH), 49.9 (+, CH), 46.5 (+, CH), 23.3 (+, 2C, CH_3), 19.3 (+, 2C, CH_3); EI (m/z , 70 eV, 80 °C): 310 (39) [M]⁺, 210 (60), 181 (13), 131 (17), 100 (48), 92 (11), 91 (100), 86 (10), 84 (14), 77 (22), 71 (12), 70 (10), 69 (35), 58 (54), 57 (23), 55 (15); HRMS ($C_{17}H_{22}N_6$): Calcd 310.1906, Found 310.1905; IR (ATR, $\bar{\nu}$) = 3122 (w), 3058 (vw), 3031 (vw), 2979 (w), 2934 (w), 2868 (vw), 2223 (m), 1816 (vw), 1700 (vw), 1604 (vw), 1537 (s), 1497 (w), 1456 (m), 1412 (vs), 1368 (vs), 1353 (s), 1326 (w), 1313 (w), 1261 (vs), 1239 (m), 1227 (vs), 1184 (w), 1149 (vs), 1132 (m), 1095 (m), 1081 (w), 1028 (s), 1001 (m), 970 (w), 909 (w), 881 (w), 851 (m), 843 (m), 819 (w), 799 (w), 752 (w), 741 (s), 721 (m), 711 (vs), 694 (s), 649 (m), 632 (w) cm^{-1} .

13a: (E)-1-benzyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-1H-pyrazole-4-carbonitrile; Formula: $C_{17}H_{22}N_6$; Exact Mass: 310.1906; Smiles: CC(N(C)C)C#N=Nc1n[nH]c1C#N; InChIKey: AQYSAAXLCHFEFGV-QZQOTICOSA-N

R_f = 0.30 (cyclohexane/ethyl acetate 4:1). 1H NMR (400 MHz, $CDCl_3$, ppm) δ = 7.65 (s, 1H), 7.35–7.21 (m, 5H), 5.36 (s, 2H), 5.16 (hept, J = 6.9 Hz, 1H), 4.08 (hept, J = 6.6 Hz, 1H), 1.44 (d, J = 6.6 Hz, 6H), 1.26 (d, J = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ = 154.8, 142.5 (+, CH), 136.5, 128.8 (+, 2C, CH), 128.0 (+, CH), 127.9 (+, 2C, CH), 116.0, 77.9, 52.3 (+, CH), 51.4 (+, CH), 48.1 (+, CH), 23.3 (+, 2C, CH_3), 19.0 (+, 2C, CH_3); EI (m/z , 70 eV, 70 °C): 311 (10) [M-H]⁺, 310 (55) [M]⁺, 210 (26), 181 (20), 131 (30), 119 (21), 100 (26), 91 (78), 69 (100), 58 (21); HRMS ($C_{17}H_{22}N_6$): Calcd 310.1906, Found 310.1905; IR (ATR, $\bar{\nu}$) = 3111 (w), 3089 (vw), 3067 (vw), 3031 (w), 2987 (w), 2975 (w), 2935 (w), 2871 (w), 2220 (s), 1761 (vw), 1606 (vw), 1533 (m), 1494 (w), 1466 (w), 1455 (m), 1441 (w), 1419 (vs), 1391 (s), 1375 (vs), 1363 (vs), 1313 (m), 1272 (s), 1238 (vs), 1211 (vs), 1164 (s), 1132 (s), 1103 (vs), 1078 (m), 1026 (vs), 946 (w), 936 (w), 909 (m), 884 (s), 850 (w), 815 (w), 785 (m), 722 (vs), 710 (s), 691 (vs), 666 (m), 630 (m), 615 (w) cm^{-1} .

Additional information on the chemical synthesis is available *via* Chemotion repository:
<https://doi.org/10.14272/reaction/SA-FUHFF-UHFFADPSC-KRKANKRSFKB-UHFFADPSC-NUHFF-NVGOA-NUHFF-ZZZ>
Additional information on the analysis of the target compound is available *via* Chemotion repository:
<https://doi.org/10.14272/AONLLYWWGOIMLR-XUTLUUPISA-N.1>
<https://doi.org/10.14272/AQYSAAXLCHFEFGV-QZQOTICOSA-N.1>

(E)-3-(3,3-diisopropyltriaz-1-en-1-yl)-1-(4-methylbenzyl)-1H-pyrazole-4-carbonitrile (12b), (E)-5-(3,3-diisopropyltriaz-1-en-1-yl)-1-(4-methylbenzyl)-1H-pyrazole-4-carbonitrile (13b)



In a vial, 5-[(E)-[di(propan-2-yl)amino]diazenyl]-1-[(H)-pyrazole-4-carbonitrile (15, 563 mg, 2.55 mmol, 1.00 equiv) was dissolved in 20 mL of DMSO. Cesium carbonate (1.00 g, 3.07 mmol, 1.20 equiv) and 1-(bromomethyl)-4-methylbenzene (700 mg, 3.78 mmol, 1.48 equiv) were added. The mixture was stirred first at 21 °C for 2 hours, then at 50 °C for 12 hours. The reaction was quenched with ice and extracted

Element: *Wellplates*

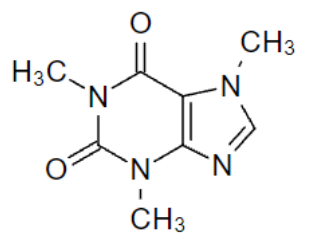
The screenshot displays the Chemotion ELN interface. On the left, a sidebar shows a collection of chemical structures and their corresponding chemical formulas: C32H46O8, C27H44O4, C25H38O5, C15H15NO2, and C24H34O4. The main area shows a wellplate design for an MTT assay. The wellplate is a 12x8 grid with columns numbered 1 to 12 and rows lettered A to H. The design includes chemical structures and color-coded wells (green, red, purple) representing different samples or conditions. The interface also includes a top navigation bar with various icons and a bottom section with buttons for 'Close', 'Save', 'Export samples', and 'Print Wells'.

- Flexibles, generisches Element um
- Verfügt über Funktionen wie:
 - Texte, Bilder oder Tabellen einfügen
 - Verlinken von *Reactions* und *Samples*
- Verlinkung von Literatur
- Hinzufügen von unterschiedlichen Anhängen
- Exportfunktionen (.docx, .odt, HTML, markdown, LaTeX)

Cell viability of HepG2 cells treated with methylxanthines

Cell viability of HepG2 cells treated with methylxanthines

Export ▾



CN1C=NC2=C1C(=O)N(C)C(=O)N2C
C₈H₁₀N₄O₂
caffeine

Sample	Dilution	Solvent [μL]	Stock solution [μM]	Volume stock [μL]	Test concentraion [μM]
caffeine	1:10	100	1000	900	100
caffeine	1:100	10	1000	990	10
caffeine	1:1000	1	1000	999	1
theobromine	1:100	20	500	480	10
theobromine	1:1000	2	500	498	1

Protocol Cell Culture:

1. Seed HepG2 cells at a concentration of 4×10^3 cells/well in 100 μl culture medium containing various amounts of the samples (final concentration e.g., 0.005 – 25 ng/ml) into microplates (tissue culture grade, 96 wells, flat bottom).
2. Incubate cells for 48 h at 37°C and 5% CO₂.
3. Add 10 μl/well Cell Proliferation Reagent WST-1 and incubate for 4 h at 37°C and 5% CO₂.
4. Shake thoroughly for 1 min on a shaker.
5. Measure the absorbance of the samples against a background control as blank using a microplate (ELISA) reader. The wavelength for

- Als weitere neue Elemente sind *Cell Lines* & *Vessel Element* im neusten Update dazu gekommen
- Für einen Einblick in alle Funktionen gibt es die Dokumentation:
<https://www.chemotion.net/docs/elc>



- Für nicht-synthese Workflows -> Erzeuge deinen eigenen Workflow

TemplatePreview

Template of Element [catch] ver.: a764d77d-4cef-4a0b-ba87-c95a99f77229 draft: dc8a99a7-f5a6-4aa9-8dc2-ca422c15be86

Layers

Reaction table for catalyst testing of type II

1 components

Characterization

1 type_char

2 type_char2

3 type_char3

Gas characterization

1 analyses

Type of experiment

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

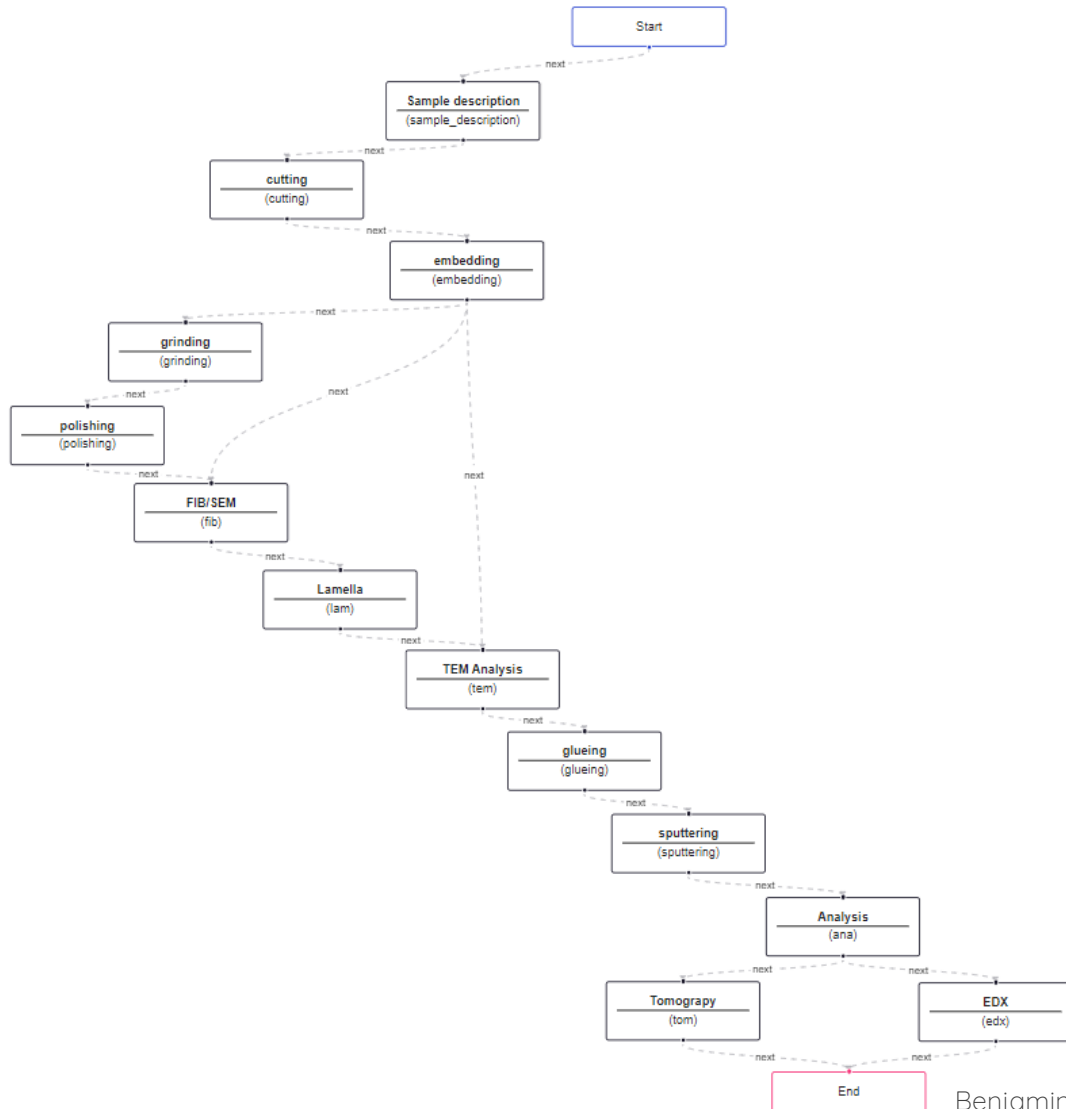
atm

LabMotion

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

Benjamin Golub *et al.* (2023) „FAIR Data Principles in NFDI – Chemotion ELN“. Zenodo, doi: [10.5281/zenodo.10014354](https://doi.org/10.5281/zenodo.10014354).

33

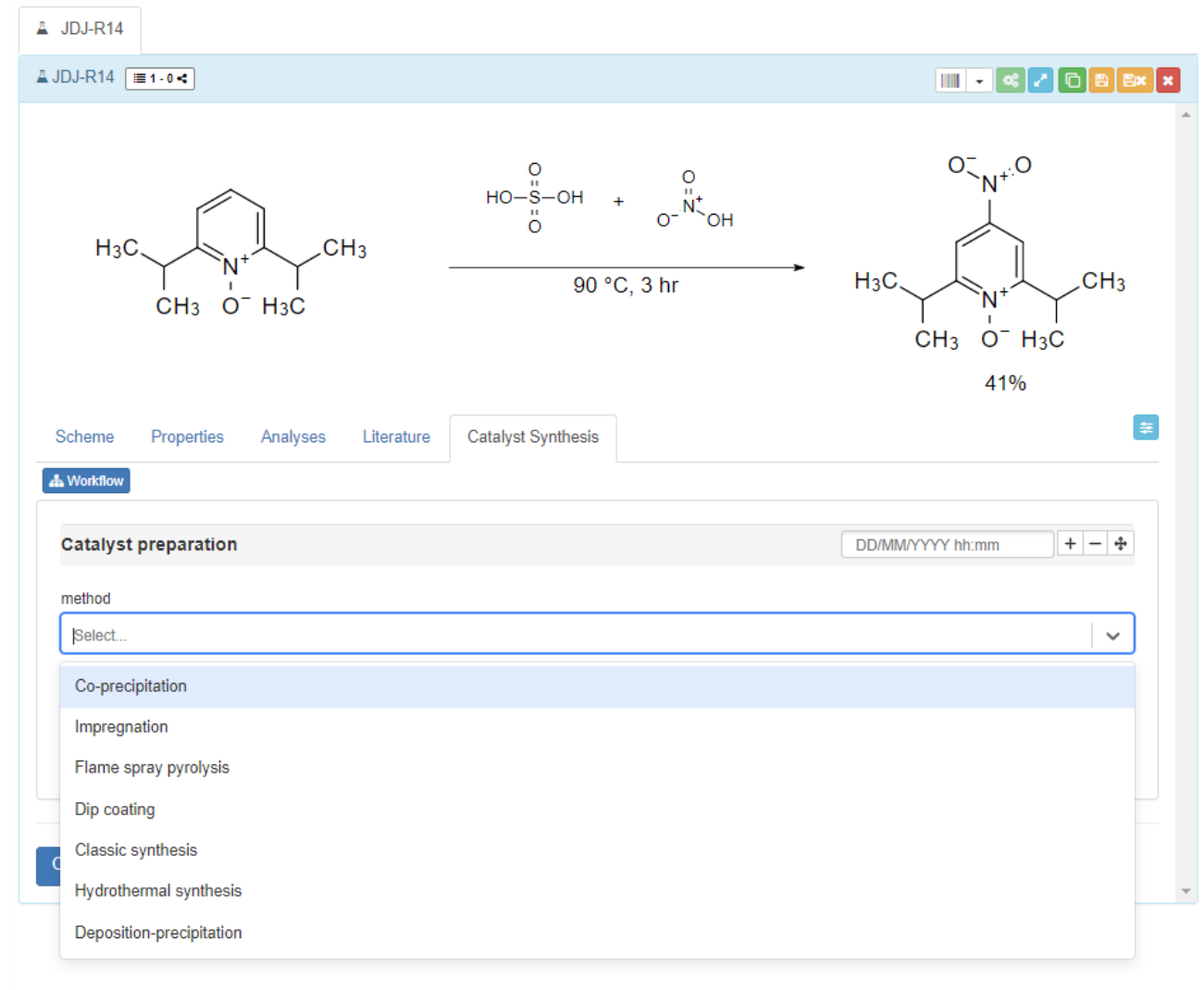


- Klare Definition von Arbeitsabläufen
- Eindeutige Vorlagen, um ein Vorgehen nach vorgegebenem Arbeitsablauf sicherzustellen
- Mehrere vordefinierte Pfade sind für eine Vorlage möglich

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- Eindeutige Vorlagen, um ein Vorgehen nach vorgegebenem Arbeitsablauf sicherzustellen
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The screenshot shows a web application window titled 'JDJ-W1 HeFDI Workflow Demo'. Inside, there's a sub-header 'JDJ-W1' with tabs for 'Properties', 'Analyses', and 'Attachments'. A 'Workflow' button is visible. Below, a text field contains 'HeFDI Workflow Demo'. A blue bar labeled 'Basic sample' with a '+' icon is present. The main form has five sections: 'Sample' with a hexagon icon, 'Material' with a red trash icon and a text input 'Test', 'Dimensions' with a text input 'XY', 'Details' with a text input 'Lorem Ipsum', and 'Next' with a 'Select...' dropdown. At the bottom are 'Close' and 'Create' buttons.

- Für vorhandene *Elemente* können zusätzliche Reiter, sogenannte *Segments*, erzeugt werden
- Zusätzliche, benutzerdefinierte *Segments* können Methoden und Arbeitsabläufe spezifisch für die Bedürfnisse Ihrer Arbeitsgruppe enthalten

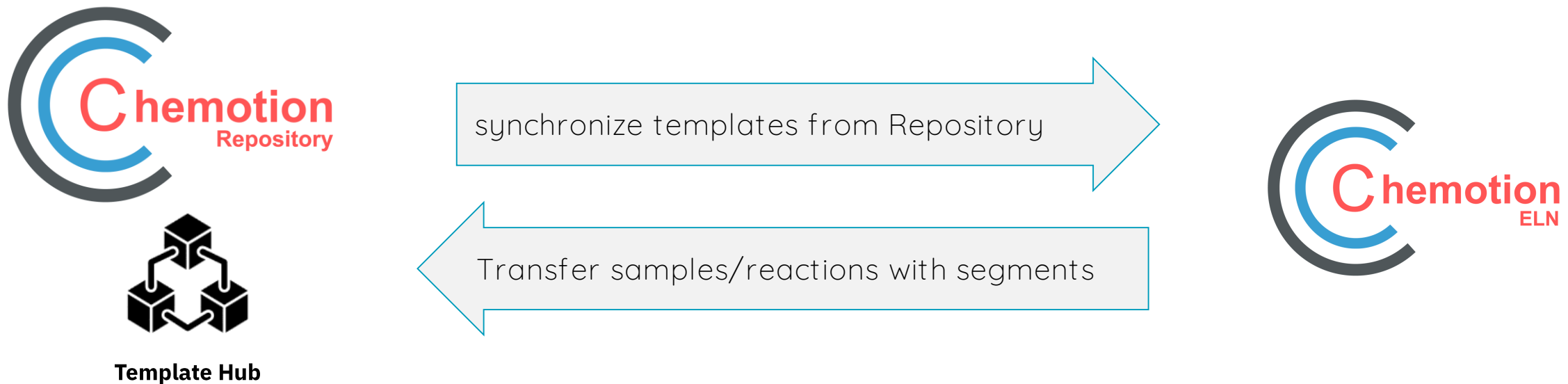


- Nur Nutzende mit der „Generic Designer“ Rolle können neue *Elements* oder *Segments* erzeugen
- Rolle kann durch Admin vergeben werden
 - Sicherung einer standardisierten Dokumentation

The screenshot displays the 'Generic Elements Designer' web interface. At the top, there are navigation links: 'Back to MyDB', 'Generic Elements Designer' (active), 'Generic Segments Designer', and 'Generic Datasets Designer'. The user is logged in as 'Benjamin Golub'. Below the navigation bar, there is a section titled 'Generic Elements Designer' with a 'Fetch from LabMotion Hub' button and a 'New Element' button. A table lists various elements with columns for Action, Active status, Name, Prefix, Element name, Icon, Description, Template, Version, Release date, Update date, ID, and Sync Time. The 'gaskk' element is highlighted. To the right, a user profile dropdown menu is open, showing options like 'Account & Profile', 'Change Password', 'My Affiliations', 'My Groups & Devices', 'My Labels', 'Converter Profile', 'My Devices', and 'Generic Designer'.

Action	Active	Name	Prefix	Element ...	Icon	Descript...	Template	Version	Release...	Update...	Id	Sync Time
		dset	DS	Device Sett...		Setting of ...			2023-01-10...	2023-01-10...	1330242d-...	
		dve	D	Device		Devices ge...			2023-01-12...	2023-01-12...	83e6796f-b...	
		echem	ELCH	eChem		echemie test			2023-07-07...	2023-09-20...	0d6c774a-c...	
		emspc	spectra	Ensemble e...		First test of...			2023-06-09...	2023-06-09...	fe1d5931-f...	
		emspe	emspec	Emission s...		Formal app...			2023-03-09...	2023-03-09...	c2acbdda-c...	
		gaskk	G	Catalysis - ...		edit Katja O...			2023-01-16...	2023-01-16...	6c4cd9ba-3...	
		gasnj	G	Catalysis - ...		edit Nicole ...			2022-11-03...	2022-11-03...	f075520e-9...	
		gene	G	Gene					2021-08-11...	2023-08-08...	46312583-...	
		gsmw	GSMW	GSMW_1-S...		Check if all...			2023-08-22...	2023-09-05...	5048a070-a...	
		gsmwb	GSMW	GSMW_2-S...		Process to ...		1.1	2023-08-24...	2023-09-01...	2b0983c6-7...	

- Veröffentlichung von und Zugriff auf generische Elements/Segments im Chemotion Repository
- Vorhandene Vorlagen, von anderen Forschenden, können nachgenutzt und müssen nicht neu erfunden werden



- Offizielle Demoinstanz: <https://demo.chemotion.ibcs.kit.edu/home>
- Es selbst lokal installieren
- Für einen leichteren Einstieg gibt es Einführungsvideos (DE/EN):
<https://www.youtube.com/@chemotioneln9781/videos>
- Bei Fragen hilft der Helpdesk von FDM-NDS gern weiter:
info@fdm-nds.de
- Oder der Helpdesk der NFDI4Chem: helpdesk@nfdi4chem.de

- Chemotion ELN wird in der Academic Cloud verfügbar sein
 - Bereitgestellt durch das Basis-Dienste-FDM Projekt
 - Betreut durch die UB der TU Braunschweig
- Wann es zugänglich sein wird, steht leider noch nicht fest

Gibt es noch Fragen?

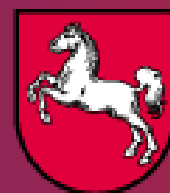


- Helpdesk von FDM-NDS: info@fdm-nds.de
- Alle Veranstaltungen von FDM-NDS:
https://fdm-nds.de/index.php/veranstaltungen_aktuell/
- Monatlicher Newsletter von FDM-NDS:
<https://fdm-nds.de/index.php/newsletter/>
- Save-the-Date: 13.-14.11.2024 Data Days Niedersachsen
 - Mehr Informationen folgen bald

**Vielen Dank für Ihre
Aufmerksamkeit!**

zukunft.
niedersachsen

Gefördert durch:



**Niedersächsisches Ministerium
für Wissenschaft und Kultur**

FDM

**Forschungsdatenmanagement
Niedersachsen**

INDS