



NFDI₄Chem

ENHANCE
YOUR
DATA.

NFDI4Chem: Chemical Research Data Management and Digital Chemistry



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

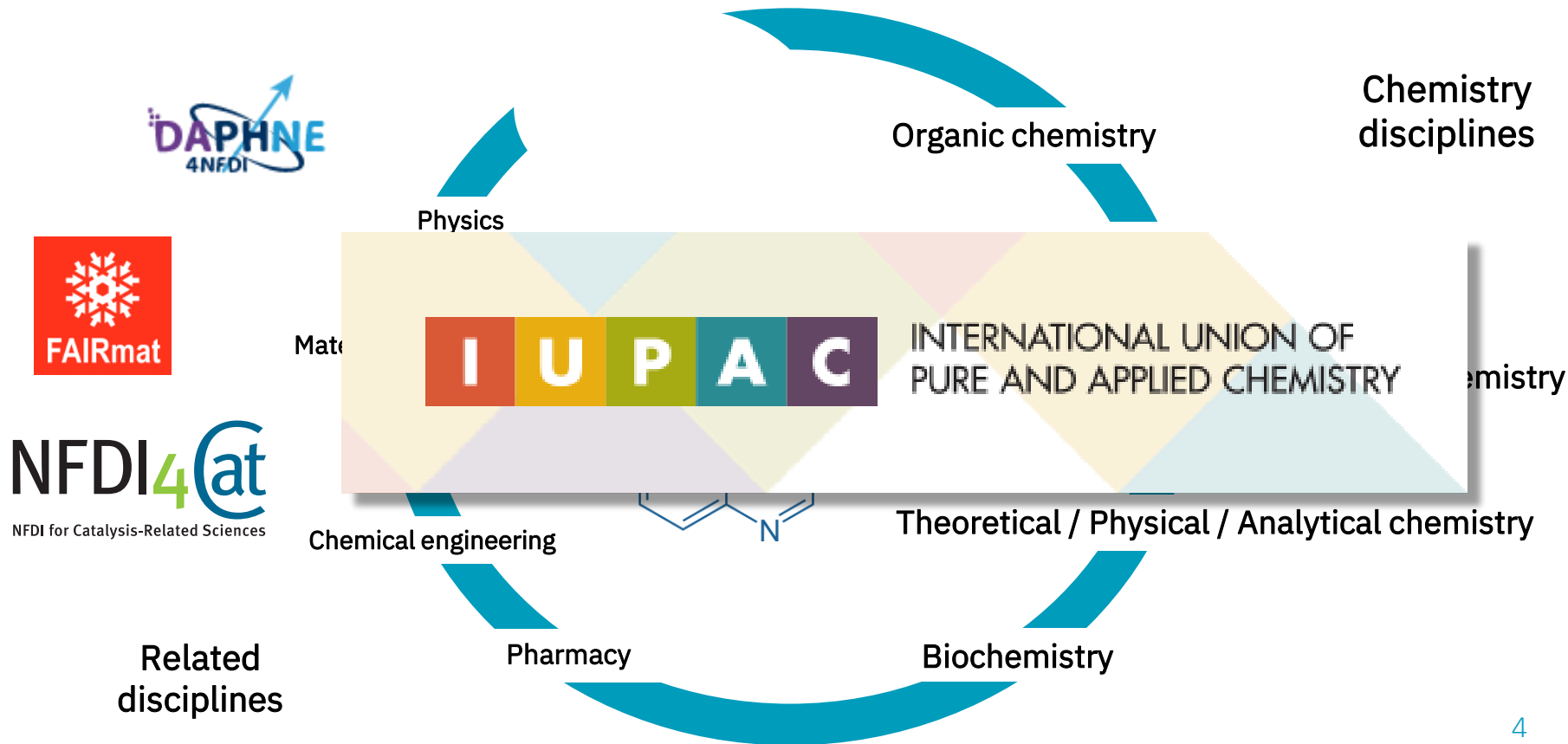
<https://www.youtube.com/watch?v=uJ01g9m8uE4>

<https://www.youtube.com/watch?v=qyKIc1crjw>

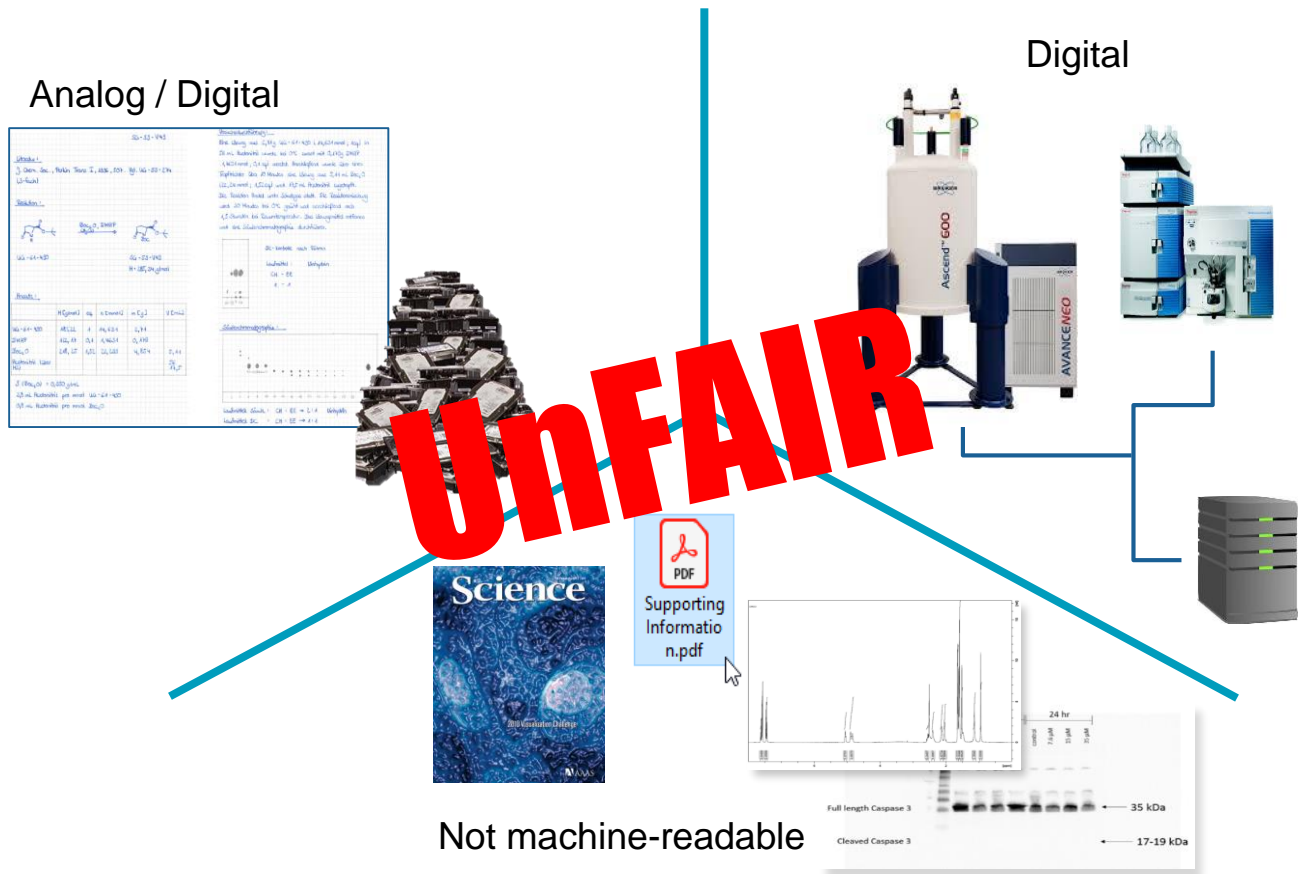
NFDI4Chem – Who we are



Our Scientific Community



Status Quo: Digital to Analog



Forces and Needs



The screenshot shows the DFG (Deutsche Forschungsgemeinschaft) website. The header includes the DFG logo and name, a search bar, and a navigation menu with links for 'Förderung', 'Geförderte Projekte', and 'DFG im Profil'. A 'DFG MAGAZIN' banner is also visible. The main content area is titled 'Information für die Wissenschaft Nr. 25 | 14. März 2022' and 'Konkretisierung der Anforderungen zum Umgang mit Forschungsdaten in Förderanträgen'. A sub-header reads 'Ausführungen in Förderanträgen werden verpflichtend'. The text discusses the requirement for a fachspezifisch adäquater Umgang mit Forschungsdaten and mentions the digital transformation in science.

DFG Deutsche Forschungsgemeinschaft

Startseite > Förderung > Ausschreibungen - Informationen für die Wissenschaft > Konkretisierung der Anforderungen zum Umgang mit Forschungsdaten in Förderanträgen

Information für die Wissenschaft Nr. 25 | 14. März 2022

Konkretisierung der Anforderungen zum Umgang mit Forschungsdaten in Förderanträgen

Ausführungen in Förderanträgen werden verpflichtend

Ein fachspezifisch adäquater Umgang mit Forschungsdaten, die wissenschaftlichen Projekten zugrunde liegen oder bei deren Durchführung entstehen, ist ein wesentlicher Bestandteil qualitätsorientierter und anschlussfähiger Forschung. Die Deutsche Forschungsgemeinschaft (DFG) konkretisiert nun die Anforderungen an den Umgang mit Forschungsdaten in den Anträgen von Einzel- und Verbundvorhaben und macht Angaben dazu verpflichtend.

Der digitale Wandel in der Wissenschaft hat den Zugang zu Forschungsdaten, die methodischen Entwicklungen zur Verarbeitung von Forschungsdaten und die Analysemethoden zur Beantwortung komplexer Forschungsfragen durch Datenmanagement stimuliert. In nahezu allen Fachbereichen ist das Bewusstsein

n of a working group:

m 10 years ago?

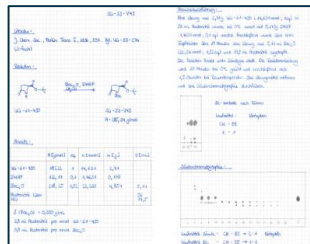
om 15 years ago?

made compound xy?

Our Focus: Molecules and Related Meta(data)



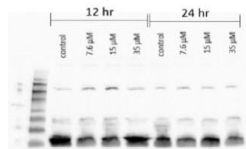
Reactions



Experimental Description
Educts / Reagents
Conditions

...

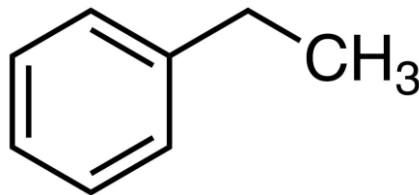
Biological activity



Organism
Conditions
Activity

...

Properties



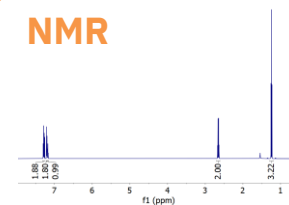
Name
Formula
CAS
InChI Key

Ethylbenzene
 C_8H_{10}
100-41-4
YNQLUTRBYVCPMQ-
UHFFFAOYSA-N

...

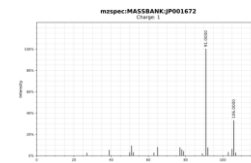
Assignment

NMR



Nucleus
Pulse sequence
Solvent ...

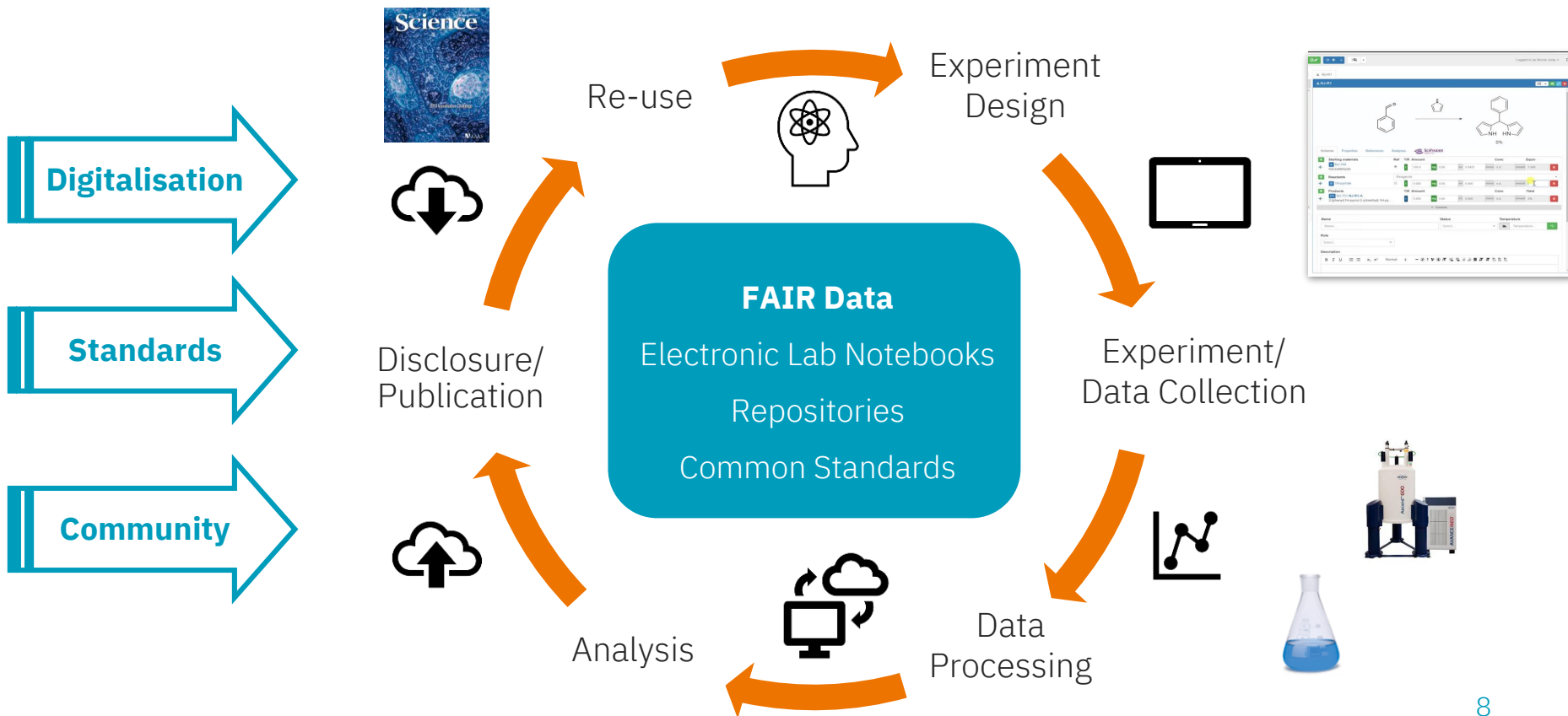
MS



Ionisation method
Voltage ...

Spectra

Our Vision

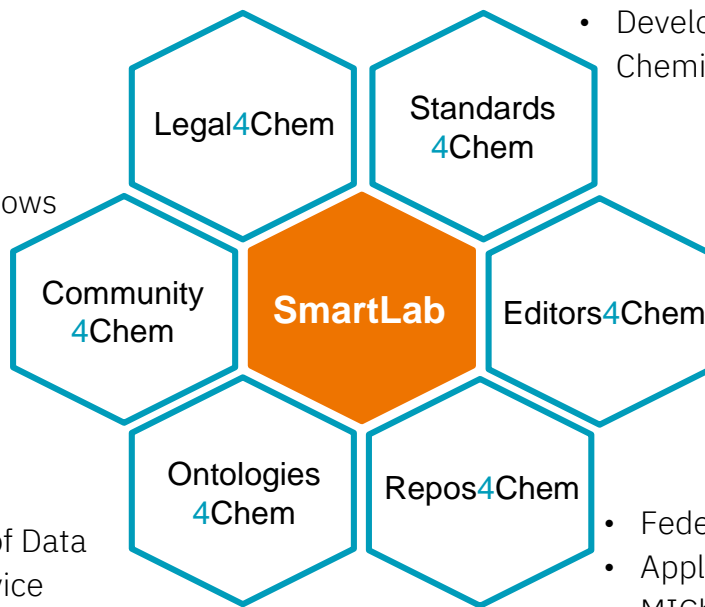




Legally reliable framework of policies and guidelines for FAIR research data management

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

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



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



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

- Federation of Repos
- Applying FAIR Data
- MICH

Smart Lab - Seamless Data Flows



Devices



Data

Electronic Lab Notebook (ELN)



Data

Federated
Repositories



ELN reporting function to generate SI

5-[4-(E)-[di(n-propan-2-ylamino)diazene]-1-yl]-pyrazole-4-carbonitrile (15)



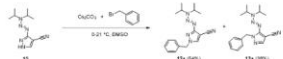
18: 5-((*E*)-[di(prop-2-yl)amino]diazene)-1-*H*-pyrazole-4-carbonitrile; Formula: $C_{10}H_{16}N_6$; Exact Mass: 220.1436; Smiles: CC(N(C)C)C(N=N)nc1cc[nH]1C#N; InChIKey: UCPMQT7XXGDIFF-CCEZHUSRA-N.

To a mixture of 5-amino-10-oxo-10H-pyran-2-carboxylic acid (2.06 g, 19 mmol, 1.00 equiv) in 6 mL of water, conc. hydrochloric acid (6.11 mL, 74 mmol, 4.00 equiv) was added. The mixture was cooled to 0 °C and a solution of sodium acetate (1.28 g, 19 mmol, 1.50 equiv) in 20 mL of water was added. Additional 10 mL of water were added to give a stirrable slurry. After stirring the 10 mm at 0 °C, a mixture of diisopropylamine (2.43 g, 1.37 mol, 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 dieneum 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 fry). 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.

[illegible]

Additional information on the chemical synthesis is available via Chemotion repository:
<https://doi.org/10.14272/reaction/5A-FUHTF-LHTFTADPSC-UCPMQTTXXM-LHTFTADPSC-SUHTF-NEHPV-SUHTF-ZZZ>
 Additional information on the analysis of the target compound is available via Chemotion repository:
<https://doi.org/10.14272/UCPMQTTXXMXHTF-CCEZHSRISA-N1>

(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-diisopropylfuryl)-1-methyl-4-cyanitrile-2H-pyrazole (15, 76.5 mg, 347 μmol , 1.00 equiv) was dissolved in 10 mL of DMSO. Cesium carbonate (133 mg, 409 μmol , 1.18 equiv) was added and the solution was cooled to 0 °C. Bromomethylbenzene (117 mg, 80.9 μL , 681 μmol , 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 \times 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-disopropylthiaz-1-en-1-yl)-5H-pyrazole-4-carbonitrile (**12a**, 58.2 mg, 188 μ mol, 54% yield) as a light-orange solid and (E)-1-benzyl-5-(3,3-disopropylthiaz-1-en-1-yl)-5H-pyrazole-4-carbonitrile (**13a**, 38.7 mg, 125 μ mol, 10% yield) as a light-orange solid.

12a. (E)-1-benzyl-3-(3,3-diisopropyltriaz-1-en-1-yl)-1H-pyrazole-4-carbonitrile, Formula: $C_{21}H_{25}N_5$, Exact Mass 310.1906, Smiles: N#Cc1cc(n1)/N=N/C(C(C)C)C(C)C, InChIKey: AONLLYWGOIMLR-XUTLITPISA-N

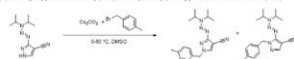
$\delta_{\text{H}} = 6.23$ (cyclohexene-ethyl acetate 4:1); ^1H NMR (400 MHz, CDCl_3 , ppm): $\delta = 7.53$ (s, 1H), 7.30–7.15 (m, 5H), 5.32 (m, 2H), 4.8–4.81 (m), 5.13 (s, 2H), 3.93 (m, 2H), 3.6–4.16 (m), 1.39 (t, 3H), $\delta_{\text{C}} = 6.6$ (H), 11.5 (t, 4), $\delta_{\text{C}} = 6.8$ (H), ^13C NMR (100 MHz, CDCl_3 , ppm): $\delta = 162.9$, 135.7, 7.9, CH_3 , 134.8, 139.1 (t, 2C), CH_2 , 128.8 (t, 2C), 128.6 (t, 2C), 128.1 (t, 2C), 127.9 (t, 2C), 127.7 (t, 2C), 127.5 (t, 2C), 127.4 (t, 2C), 127.3 (t, 2C), 127.2 (t, 2C), 127.1 (t, 2C), 127.0 (t, 2C), 126.9 (t, 2C), 126.8 (t, 2C), 126.7 (t, 2C), 126.6 (t, 2C), 126.5 (t, 2C), 126.4 (t, 2C), 126.3 (t, 2C), 126.2 (t, 2C), 126.1 (t, 2C), 126.0 (t, 2C), 125.9 (t, 2C), 125.8 (t, 2C), 125.7 (t, 2C), 125.6 (t, 2C), 125.5 (t, 2C), 125.4 (t, 2C), 125.3 (t, 2C), 125.2 (t, 2C), 125.1 (t, 2C), 125.0 (t, 2C), 124.9 (t, 2C), 124.8 (t, 2C), 124.7 (t, 2C), 124.6 (t, 2C), 124.5 (t, 2C), 124.4 (t, 2C), 124.3 (t, 2C), 124.2 (t, 2C), 124.1 (t, 2C), 124.0 (t, 2C), 123.9 (t, 2C), 123.8 (t, 2C), 123.7 (t, 2C), 123.6 (t, 2C), 123.5 (t, 2C), 123.4 (t, 2C), 123.3 (t, 2C), 123.2 (t, 2C), 123.1 (t, 2C), 123.0 (t, 2C), 122.9 (t, 2C), 122.8 (t, 2C), 122.7 (t, 2C), 122.6 (t, 2C), 122.5 (t, 2C), 122.4 (t, 2C), 122.3 (t, 2C), 122.2 (t, 2C), 122.1 (t, 2C), 122.0 (t, 2C), 121.9 (t, 2C), 121.8 (t, 2C), 121.7 (t, 2C), 121.6 (t, 2C), 121.5 (t, 2C), 121.4 (t, 2C), 121.3 (t, 2C), 121.2 (t, 2C), 121.1 (t, 2C), 121.0 (t, 2C), 120.9 (t, 2C), 120.8 (t, 2C), 120.7 (t, 2C), 120.6 (t, 2C), 120.5 (t, 2C), 120.4 (t, 2C), 120.3 (t, 2C), 120.2 (t, 2C), 120.1 (t, 2C), 120.0 (t, 2C), 119.9 (t, 2C), 119.8 (t, 2C), 119.7 (t, 2C), 119.6 (t, 2C), 119.5 (t, 2C), 119.4 (t, 2C), 119.3 (t, 2C), 119.2 (t, 2C), 119.1 (t, 2C), 119.0 (t, 2C), 118.9 (t, 2C), 118.8 (t, 2C), 118.7 (t, 2C), 118.6 (t, 2C), 118.5 (t, 2C), 118.4 (t, 2C), 118.3 (t, 2C), 118.2 (t, 2C), 118.1 (t, 2C), 118.0 (t, 2C), 117.9 (t, 2C), 117.8 (t, 2C), 117.7 (t, 2C), 117.6 (t, 2C), 117.5 (t, 2C), 117.4 (t, 2C), 117.3 (t, 2C), 117.2 (t, 2C), 117.1 (t, 2C), 117.0 (t, 2C), 116.9 (t, 2C), 116.8 (t, 2C), 116.7 (t, 2C), 116.6 (t, 2C), 116.5 (t, 2C), 116.4 (t, 2C), 116.3 (t, 2C), 116.2 (t, 2C), 116.1 (t, 2C), 116.0 (t, 2C), 115.9 (t, 2C), 115.8 (t, 2C), 115.7 (t, 2C), 115.6 (t, 2C), 115.5 (t, 2C), 115.4 (t, 2C), 115.3 (t, 2C), 115.2 (t, 2C), 115.1 (t, 2C), 115.0 (t, 2C), 114.9 (t, 2C), 114.8 (t, 2C), 114.7 (t, 2C), 114.6 (t, 2C), 114.5 (t, 2C), 114.4 (t, 2C), 114.3 (t, 2C), 114.2 (t, 2C), 114.1 (t, 2C), 114.0 (t, 2C), 113.9 (t, 2C), 113.8 (t, 2C), 113.7 (t, 2C), 113.6 (t, 2C), 113.5 (t, 2C), 113.4 (t, 2C), 113.3 (t, 2C), 113.2 (t, 2C), 113.1 (t, 2C), 113.0 (t, 2C), 112.9 (t, 2C), 112.8 (t, 2C), 112.7 (t, 2C), 112.6 (t, 2C), 112.5 (t, 2C), 112.4 (t, 2C), 112.3 (t, 2C), 112.2 (t, 2C), 112.1 (t, 2C), 112.0 (t, 2C), 111.9 (t, 2C), 111.8 (t, 2C), 111.7 (t, 2C), 111.6 (t, 2C), 111.5 (t, 2C), 111.4 (t, 2C), 111.3 (t, 2C), 111.2 (t, 2C), 111.1 (t, 2C), 111.0 (t, 2C), 110.9 (t, 2C), 110.8 (t, 2C), 110.7 (t, 2C), 110.6 (t, 2C), 110.5 (t, 2C), 110.4 (t, 2C), 110.3 (t, 2C), 110.2 (t, 2C), 110.1 (t, 2C), 110.0 (t, 2C), 109.9 (t, 2C), 109.8 (t, 2C), 109.7 (t, 2C), 109.6 (t, 2C), 109.5 (t, 2C), 109.4 (t, 2C), 109.3 (t, 2C), 109.2 (t, 2C), 109.1 (t, 2C), 109.0 (t, 2C), 108.9 (t, 2C), 108.8 (t, 2C), 108.7 (t, 2C), 108.6 (t, 2C), 108.5 (t, 2C), 108.4 (t, 2C), 108.3 (t, 2C), 108.2 (t, 2C), 108.1 (t, 2C), 108.0 (t, 2C), 107.9 (t, 2C), 107.8 (t, 2C), 107.7 (t, 2C), 107.6 (t, 2C), 107.5 (t, 2C), 107.4 (t, 2C), 107.3 (t, 2C), 107.2 (t, 2C), 107.1 (t, 2C), 107.0 (t, 2C), 106.9 (t, 2C), 106.8 (t, 2C), 106.7 (t, 2C), 106.6 (t, 2C), 106.5 (t, 2C), 106.4 (t, 2C), 106.3 (t, 2C), 106.2 (t, 2C), 106.1 (t, 2C), 106.0 (t, 2C), 105.9 (t, 2C), 105.8 (t, 2C), 105.7 (t, 2C), 105.6 (t, 2C), 105.5 (t, 2C), 105.4 (t, 2C), 105.3 (t, 2C), 105.2 (t, 2C), 105.1 (t, 2C), 105.0 (t, 2C), 104.9 (t, 2C), 104.8 (t, 2C), 104.7 (t, 2C), 104.6 (t, 2C), 104.5 (t, 2C), 104.4 (t, 2C), 104.3 (t, 2C), 104.2 (t, 2C), 104.1 (t, 2C), 104.0 (t, 2C), 103.9 (t, 2C), 103.8 (t, 2C), 103.7 (t, 2C), 103.6 (t, 2C), 103.5 (t, 2C), 103.4 (t, 2C), 103.3 (t, 2C), 103.2 (t, 2C), 103.1 (t, 2C), 103.0 (t, 2C), 102.9 (t, 2C), 102.8 (t, 2C), 102.7 (t, 2C), 102.6 (t, 2C), 102.5 (t, 2C), 102.4 (t, 2C), 102.3 (t, 2C), 102.2 (t, 2C), 102.1 (t, 2C), 102.0 (t, 2C), 101.9 (t, 2C), 101.8 (t, 2C), 101.7 (t, 2C), 101.6 (t, 2C), 101.5 (t, 2C), 101.4 (t, 2C), 101.3 (t, 2C), 101.2 (t, 2C), 101.1 (t, 2C), 101.0 (t, 2C), 100.9 (t, 2C), 100.8 (t, 2C), 100.7 (t, 2C), 100.6 (t, 2C), 100.5 (t, 2C), 100.4 (t, 2C), 100.3 (t, 2C), 100.2 (t, 2C), 100.1 (t, 2C), 100.0 (t, 2C), 99.9 (t, 2C), 99.8 (t, 2C), 99.7 (t, 2C), 99.6 (t, 2C), 99.5 (t, 2C), 99.4 (t, 2C), 99.3 (t, 2C), 99.2 (t, 2C), 99.1 (t, 2C),

15a (E)-1-benzyl-5-(3,3-dipropyl-1H-pyrazol-1-en-1-yl)-1H-pyrazol-4-carbonitrile, Formula: $C_{21}H_{22}N_6$, Exact Mass: 310.1906, Smiles: CC(C)(C)N=N(c1cc(C#N)nn1)C2=CC=CC=C2, InChIKey: AQYSAXXLCHFEV-
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[illegible]

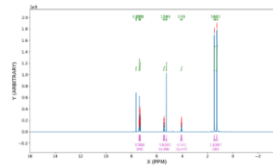
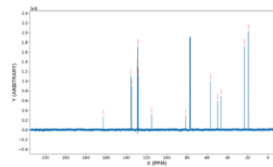
Additional information on the chemical synthesis is available via Chemotion repository:
<https://doi.org/10.14272/reaction/5A-F3E5F7-5E7FFADPSC-KKKANRSEK-UHFFFAADPSC-N3E7F-NVGOA-NUHET-ZZZ>
 Additional information on the analysis of the target compound is available via Chemotion repository:
<https://doi.org/10.14272/AONLLYYWGOMLR-XQUTUUPSA-N-1>
<https://doi.org/10.14272/AQYSAXCLCHEFFG-QOOTHROSA-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-ylamino)disilyl]-1-[H]-pyrazole-4-carbonitrile (**15**, 561 mg, 2.55 mmol, 1.00 equiv) was dissolved in 20 mL of DMSO. The solution was cooled to 0 °C. 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

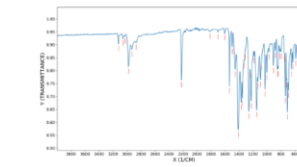
[12a] (E)-1-benzyl-3-(3,3-diisopropyltriaz-1-en-1-yl)-1H-pyrazole-4-carbonitrile

CJMO-0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)CSEM-0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)

CEMO-0000470 | mass spectrometry (MS)



CIMO-0000630 | infrared absorption spectroscopy (IR)





Dalton Transactions

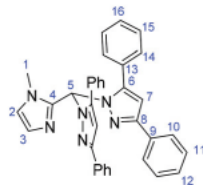
PAPER



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Cite this: DOI: 10.1039/d1dt00832c

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



^1H NMR (CD_2Cl_2 , 400 MHz): δ = 7.80 (d, 3J = 7.8 Hz, 4H, H-10), 7.67 (s, 1H, H-5), 7.39 (t, 3J = 7.4 Hz, 4H, H-11), 7.32 (d, 3J = 7.3 Hz, 4H, H-12 + H-16), 7.27 (t, 3J = 7.3 Hz, 4H, H-15), 7.12 (d, 3J = 7.1 Hz, 4H, H-14), 6.94 (d, 3J = 3.1 Hz, 2H, H-2 + H-3), 6.65 (s, 2H, H-7), 3.70 (s, 3H, H-1) ppm. **^{13}C { ^1H } 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%, $^{12}\text{C}_{35}^{1}\text{H}_{29}^{14}\text{N}_6^+$), 534.24872 (38%, $^{12}\text{C}_{34}^{13}\text{C}^1\text{H}_{29}^{14}\text{N}_6^+$), 535.25207 (7%, $^{12}\text{C}_{33}^{13}\text{C}_2^1\text{H}_{29}^{14}\text{N}_6^+$), 536.25543 (1%, $^{12}\text{C}_{32}^{13}\text{C}_3^1\text{H}_{29}^{14}\text{N}_6^+$). **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), 732 (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/LSGGPBYYVWWQPOY-UHFFFAOYSA-N.1>

nitrenes were obtained by the reaction of a copper(II) acetonitrile complex with $^5\text{PhINTs}$ in dichloromethane.



ROYAL SOCIETY
OF CHEMISTRY

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View Journal

Copper nitrenes and amination

ai C. Göbgen,
mann and

as intermediates in the copper catalyzed amination of α -haloalkanes. The copper complexes were synthesized at low temperatures. The copper (pyrazolyl)methane family. The copper

Chemotion Repository

www.chemotion-repository.net/mydb/collection/2171/sample/49359

Repository

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My Data

FT-17

C28H38N5

FT-22

C28H37Cu2F12N10P2

C12H11N5
2-[di(pyrazol-1-yl)methyl]pyridine

FT-15

C38H38N8
1-[(3,5-diphenylpyrazol-1-yl)-(1-methylimidazol-2-yl)methyl]-3,5-diphenylpyrazole

FT-7

C38H38ClN8
2-[bis(3,5-diphenylpyrazol-1-yl)methyl]-4-chloropyridine

FT-6

C28H32CuF9N9P
acetonitrile,2-[bis(3-phenylpyrazol-1-yl)methyl]pyridine,copper(1+),hexafluorophosphate

FT-5

C70H66Cu2F12N12P2
copper(1+),1,4-(3,5-diphenylpyrazol-1-yl)-1-methylimidazol-2-yl)methyl-3,5-diphenylpyrazole

FT-5

C28H32CuF9N9P
acetonitrile,2-[bis(3-phenylpyrazol-1-yl)methyl]pyridine,copper(1+),hexafluorophosphate
627.003260 g/mol
Exact mass: 626.084373 g/mol

Properties Analyses QC & curation Literature Results

Molecule C28H32CuF9N9P Stereo Abs any Stereo Rel any ☐ Top secret

Name External label Solvent

Amount 0.000 0.0000 0.000 Boiling point °C

Density Molarity Purity Melting point °C

0.0000 1.0000

Solvents

Description

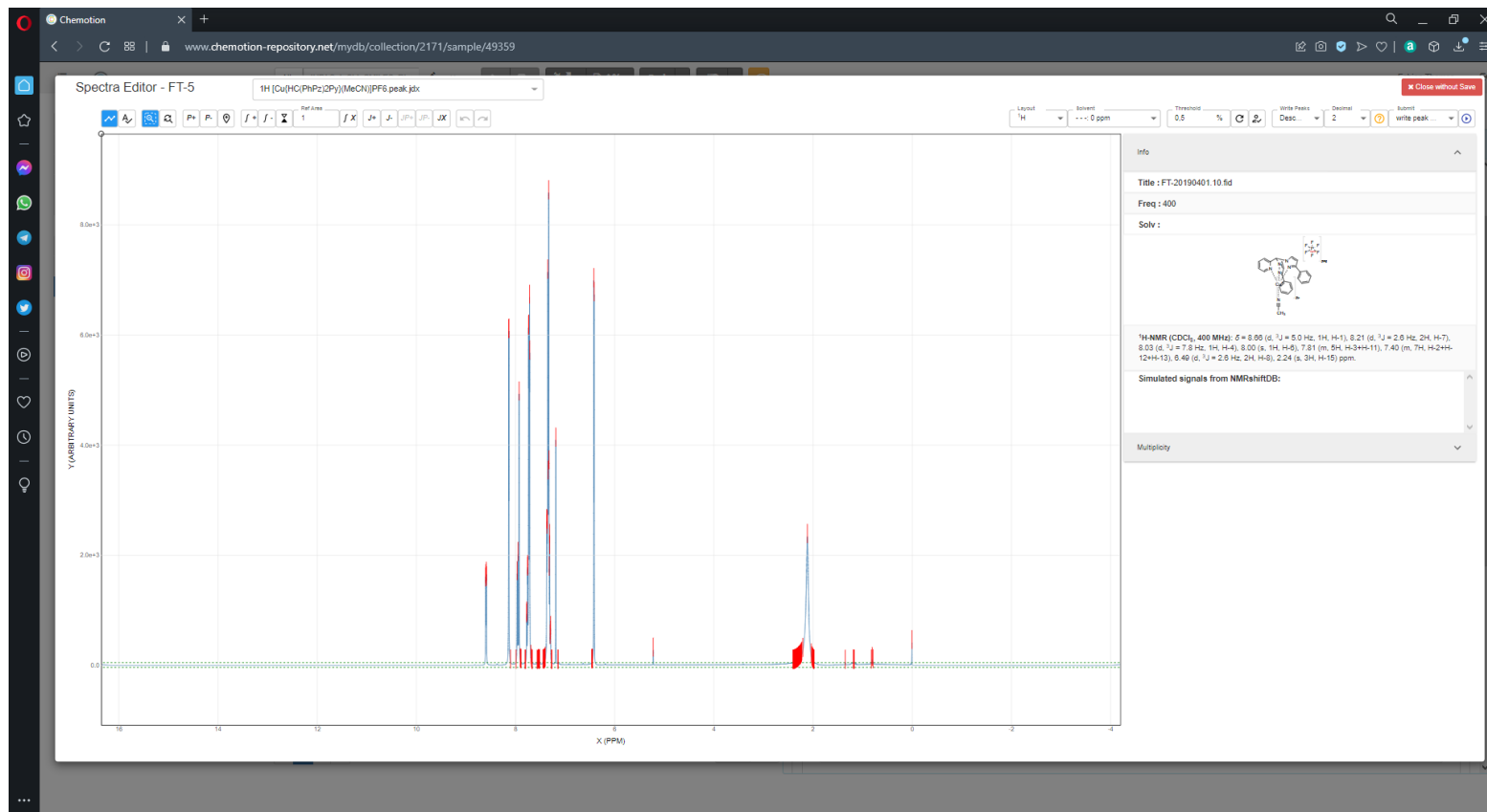
Location

Elemental composition

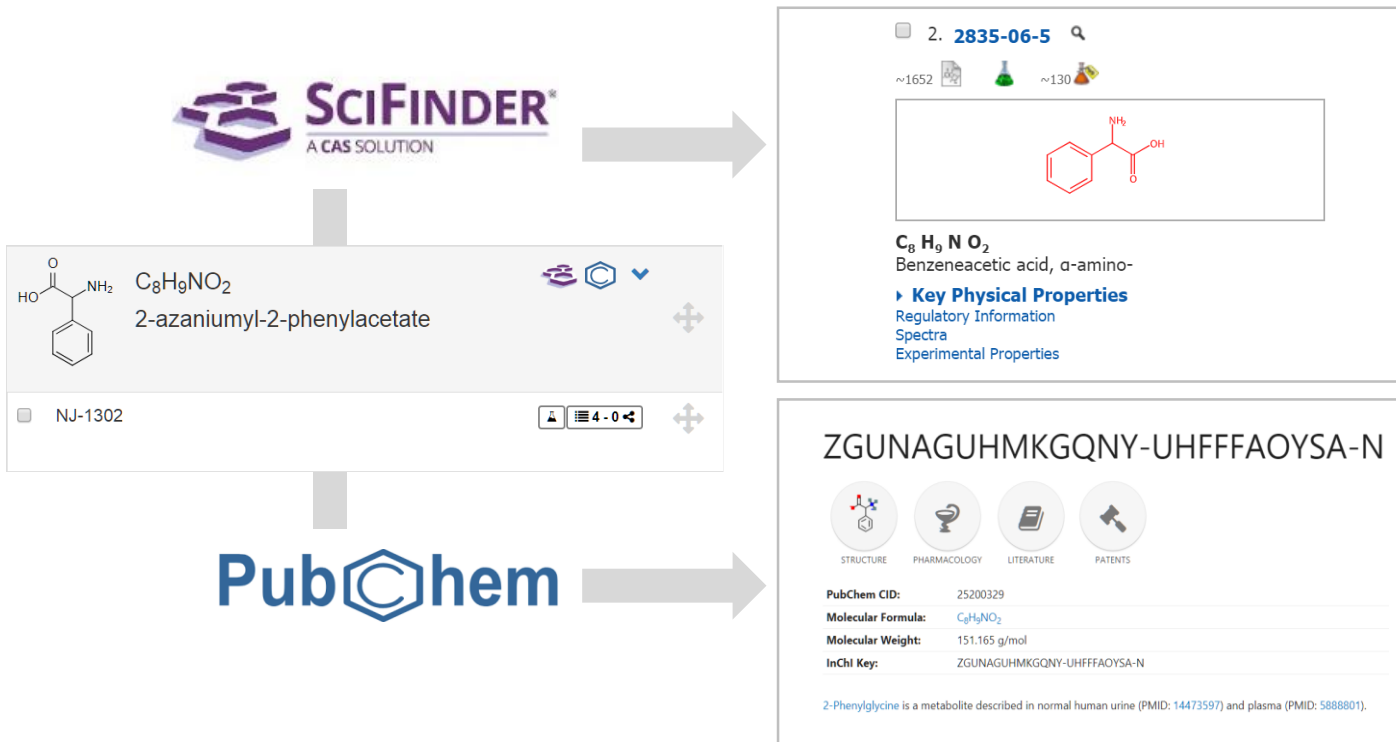
Chemical identifiers

Close Save Download Analysis

Show 15



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>

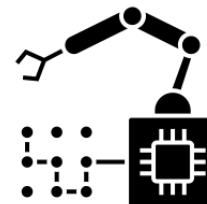
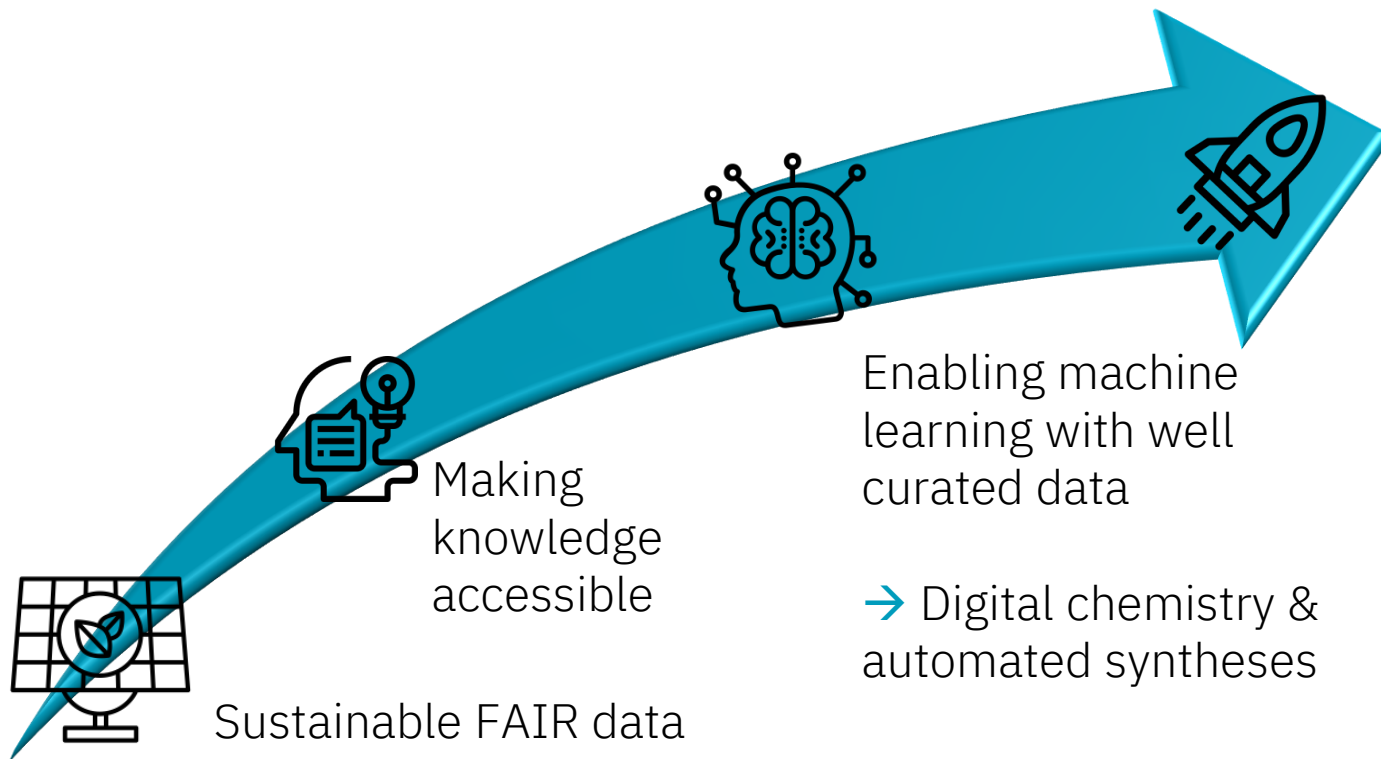


- Hosted at FSU Jena
- Free for the community
- NMR data welcome
- With generated doi and full metadata
- Direct transfer from Chemotion ELN

<https://docs.nmrxiv.org/>

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

On the way to digital chemistry



Involvement of the Community



Community requirements

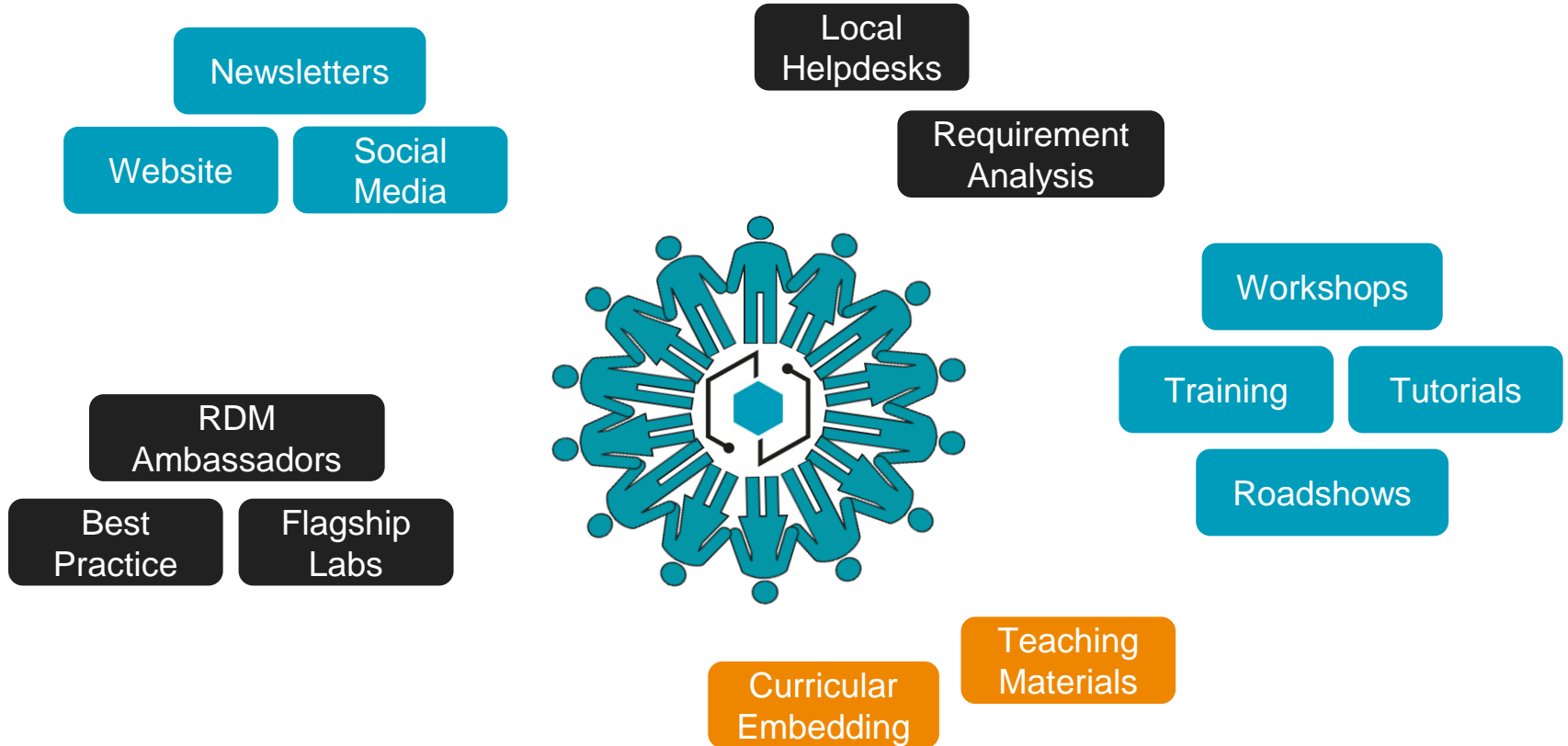


Fostering cultural change

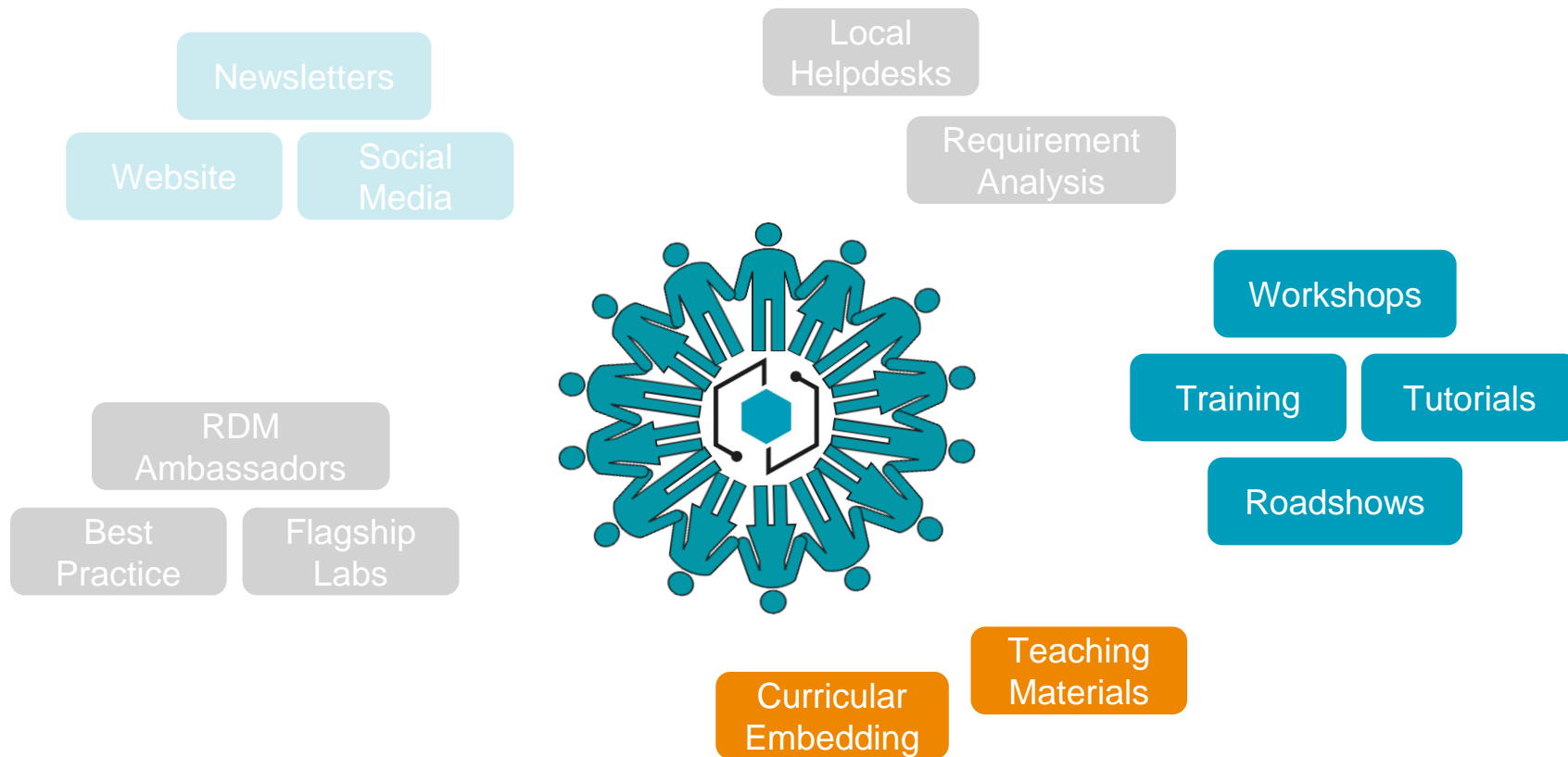
Raising RDM awareness

RDM
Infrastructure

Involvement of the Community



Involvement of the Community



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_un
d_Informationen/Downloads/Schule_Studium/PDF/2
021_GDCh_Studienkommission_Druckversion.pdf](https://www.gdch.de/fileadmin/downloads/Service_un_d_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

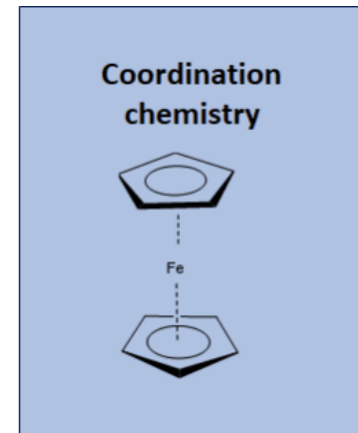
Integration into Curricular Teaching – Example 2

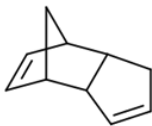
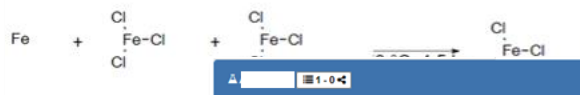


Faster way: Pre-integration into content of running lectures

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





180

Scheme	Properties	References	Analyses
--------	------------	------------	----------

Starting materials

Ref	T/R Amount
-----	------------

10



✦

| tricyclo[5.2.1.0^{2,6}]deca-3,8-diene | 147.0 |

1

Reactants

Products	T/R Amount
----------	------------

1

P1

1

cyclopenta-1,3-diene

1

P2

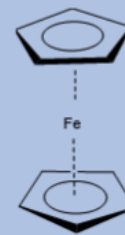
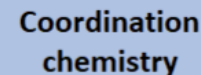
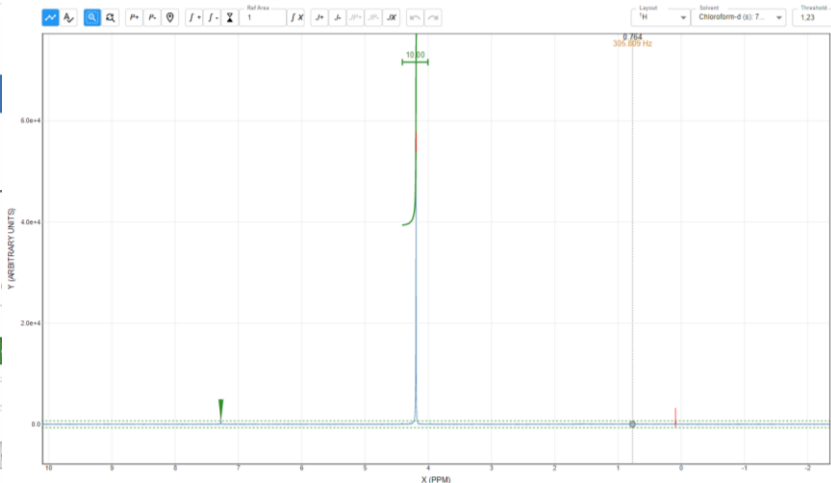
•

cyclopenta-1,3-diene

1



Default solvents	I/R	Label



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#.YjDgfTUxIPZ>

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](https://doi.org/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



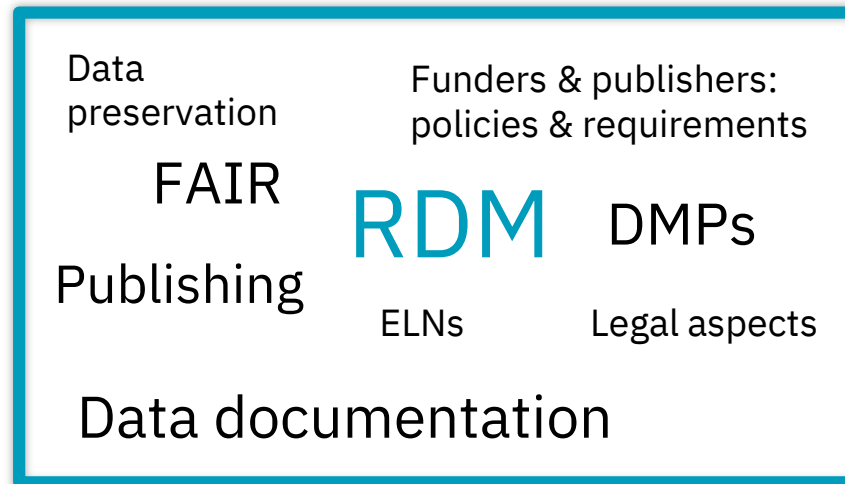
Costs: Free

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

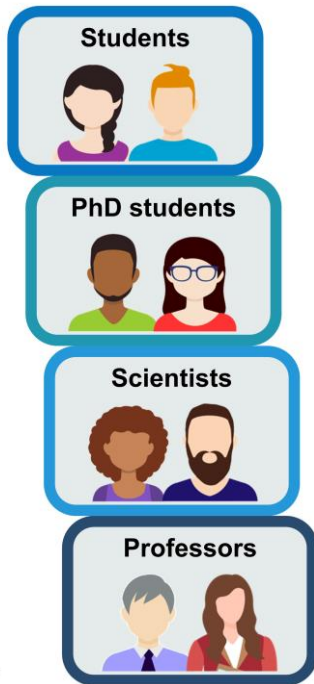


Upon request, in-person workshops at institutions

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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NFDI4Chem Knowledge Base

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

[Get started](#)



Roles



Domains



Handling Data



Topics & Concepts



Lead by Example

Funded by
DFG Deutsche
Forschungsgemeinschaft
German Research Foundation

NFDI4Chem is funded by DFG
Project Number 441958208

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[FAIR Data Principles](#)

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[Data Format Standard](#)

[Ontology](#)

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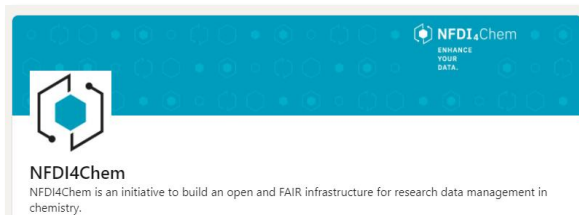
[Twitter](#)



[LinkedIn](#)

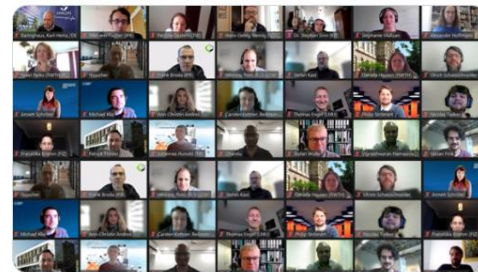


[YouTube](#)



NFDI4Chem @Nfdi4Chem · Oct 20

Last week we had our annual consortium meeting. Big thanks to all members of our advisory boards for attending & sharing their valuable insights & to all speakers for their contributions. It was amazing to see such passionate talks about solutions for [#RDM](#) in [#Chemistry](#). [@NFDI.de](#)



5 14

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 practices 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!



Subscribe to our newsletter which is released every quarter!

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Friedrich-Schiller-University Jena

Nicole Jung

Karlsruhe Institute of Technology (KIT)

Matthias Razum

FIZ Karlsruhe - Leibniz Institute for Information
Infrastructure

Johannes Liermann

Johannes Gutenberg University Mainz

Oliver Koepler*

TIB Leibniz Information Centre of Science and Technology

Sonja Herres-Pawlis

RWTH Aachen University

Felix Bach

FIZ Karlsruhe - Leibniz Institute for Information
Infrastructure

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NFDI₄Chem
ENHANCE
YOUR
DATA!



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Research Foundation) – 441958208