



NFDI₄Chem

ENHANCE
YOUR
DATA.

NFDI4Chem - Digitising Research Workflows in Chemistry

Nicole Jung, John Jolliffe

HeFDI Data Talk| 2021-12-03

Overview



- 1) NFDI and NFDI4Chem
- 2) Status Quo – What is our mission?
- 3) What is our Strategy?
- 4) What do we offer?



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YOUR
DATA.



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DATA.

NFDI and NFDI4Chem

The NFDI in General



Federal Government and the States decided to fund a [National Research Data Infrastructure](#) for Germany

- Nationale Forschungsdateninfrastruktur (NFDI)
- Funding Horizon 5y + 5y + X
- 90 Mio Euro funding in total, €70 Mio direct costs/5 years
- Eventually, 30 consortia in all areas of science funded
- €5 Mio max per consortium per year
- De-facto €2.3 Mio per year on average per consortium
- Process not competitive within each area of science!

nfdi
Nationale
Forschungsdaten
Infrastruktur

NFDI4Cat
NFDI for Catalysis-Related Sciences

Data))((PLANT


NFDI4ing


NFDI4
BIODIVERSITY

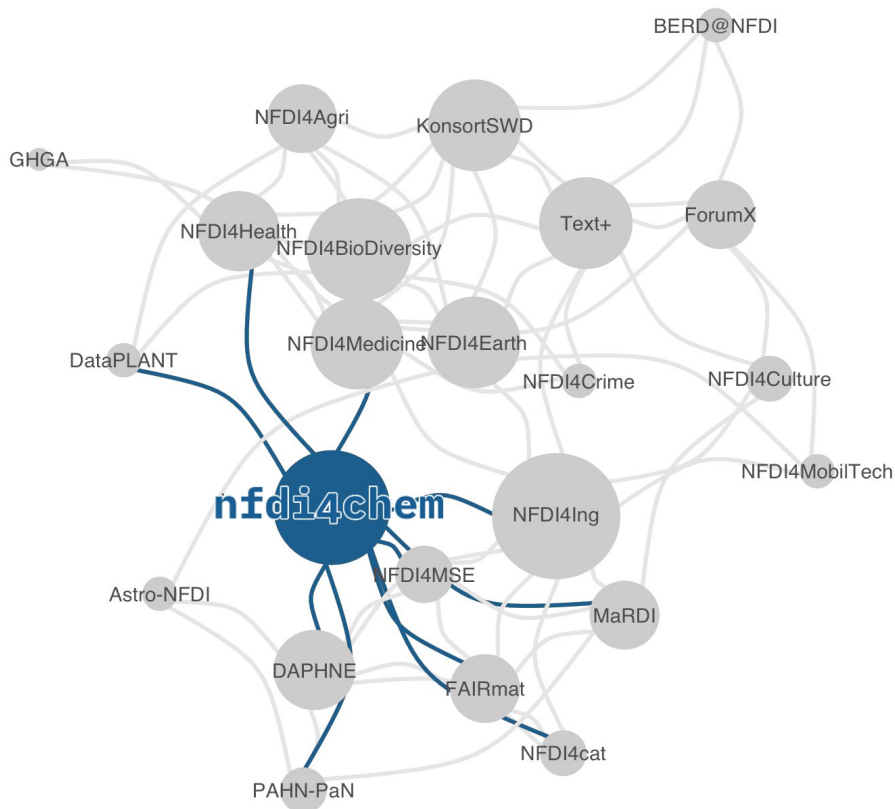
GXGA


The NFDI in General



Aus dem Koalitionsvertrag: "Das ungenutzte Potential, das in zahlreichen Forschungsdaten liegt, wollen wir effektiver für innovative Ideen nutzen. Den Zugang zu Forschungsdaten für öffentliche und private Forschung wollen wir mit einem Forschungsdatengesetz umfassend verbessern sowie vereinfachen und führen Forschungsklauseln ein. Open Access wollen wir als gemeinsamen Standard etablieren. Wir setzen uns für ein wissenschaftsfreundlicheres Urheberrecht ein. Die Nationale Forschungsdateninfrastruktur wollen wir weiterentwickeln und einen Europäischen Forschungsdatenraum vorantreiben. Datenteilung von vollständig anonymisierten und nicht personenbezogenen Daten für Forschung im öffentlichen Interesse wollen wir ermöglichen."

Embedding within the NFDI



- Molecule data as linking element between consortia
- Cooperations on chemistry related cross-cutting topics
- Collaboration on generic cross-cutting topics defined in Berlin Declaration



NFDI4Chem is embedded in an international context



Composition of the consortium



- Learned Societies



Deutsche Bunsen-Gesellschaft
für physikalische Chemie e.V.



GESELLSCHAFT
DEUTSCHER CHEMIKER



DPhG

Deutsche Pharmazeutische Gesellschaft e.V.



Composition of the consortium



- Learned Societies
- Research Data Infrastructure



Deutsche Bunsen-Gesellschaft
für physikalische Chemie



GESELLSCHAFT
DEUTSCHER CHEMI



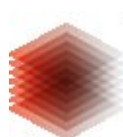
DPhG

Deutsche Pharmazeutische Gesellschaft e.V.



FIZ Karlsruhe

Leibniz Institute for Information Infrastructure



TIB



BAM



Steinbuch Centre
for Computing



Messen • Forschen • Wissen



Composition of the consortium



- Learned Societies
- Research Data Infrastructure
- Research Community



Deutsche Bunsen-Gesellschaft
für physikalische Chemie



GESELLSCHAFT
DEUTSCHER CHEMI



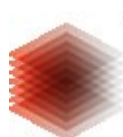
DPhG

Deutsche Pharmazeutische Gesellschaft e.V.



FIZ Karlsruhe

Leibniz Institute for Information Infrastructure



TIB



BAM



Steinbuch Centre
for Computing



Messen • Forschen • Wissen



Composition of the consortium



Deutsche Bunsen-Gesellschaft für physikalische Chemie



GESELLSCHAFT DEUTSCHER CHEMIE

UNIVERSITÄT GREIFSWALD
Wissen lockt. Seit 1456



Deutsche Pharmazeutische Gesellschaft e.V.



Christian-Albrechts-Universität zu Kiel



Leibniz Institute for Information Infrastructure





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Status Quo

Why? What is our mission?

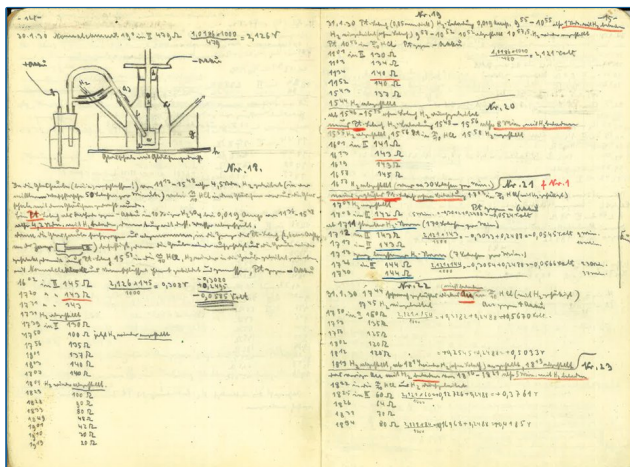


2017



iPhone 8
325.0 GFlops
2.39 GHz CPU Speed

1927



2021

Vorsuchsbeschreibung:

Eine Lösung aus 2,1g UG-64-430 (4,463 mmol; 4,4g) in 56 ml Acetonitril wurde bei 0°C mit 1 ml 2,4-DHP (1,463 mmol; 0,4 g) versetzt. Nachfolgend wurde über einen Tropftrichter über 10 Minuten eine Lösung aus 5,44 ml SnCl_4 (22,24 mmol; 4,55 g) und 187 ml Acetonitril zugegeben.

Die Reaktion wurde unter Schütteln durchgeführt. Die Reaktionsmischung wurde 30 Minuten bei 0°C gerührt und anschließend nach 4,5 Stunden bei Raumtemperatur. Das Lösungsmittel entfernten und die Säulenchromatographie durchführten.

Reaktion:

UG-64-430 $\xrightarrow[\text{Schütteln}]{\text{SnCl}_4, 2,4\text{DHP}}$ SG-53-V45

UG-64-430 SG-53-V45
H: 285,34 g/mol

Probe:

	H (g/mol)	q	n (mmol)	m (g)	V (ml)
UG-64-430	185,22	1	4,463	2,1	
2,4DHP	122,17	0,4	4,463	0,49	
SnCl_4	260,52	1,52	22,233	4,85	
Acetonitril (Lösungsmittel)					56
					187

3 (SnCl_4) = 0,850 g/ml

3,8 ml Acetonitril pro mmol UG-64-430

0,8 ml Acetonitril pro mmol SnCl_4

Säulenchromatographie:

SG-53-V45

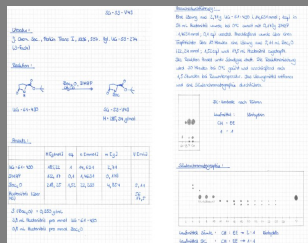
Laufmittel: CH:EE = 2:1

Laufmittel: CH:EE = 1:1

Molecules and related meta(data)

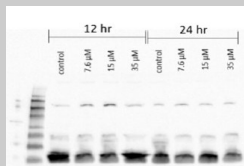


Reactions



Experimental Description
Educts / Reagents
Conditions
 ...

Biological activity



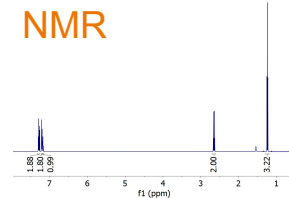
Organism
Conditions
Activity
 ...

Properties

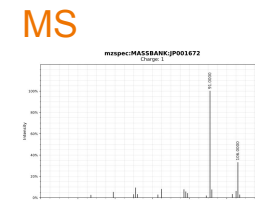
Name
 Formula
 CAS
 InChI Key
 ...

Ethylbenzene
 C₈H₁₀
 100-41-4
 YNQLUTRBYVCPMQ-
 UHFFFAOYSA-N

Assignment



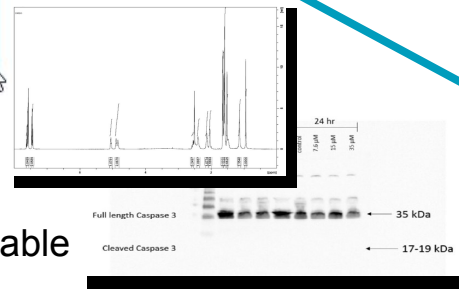
Nucleus
Pulse sequence
Solvent ...



Ionisation method
Voltage ...

Spectra

Digital



Not machine-readable

Findable
Accessible
Interoperable
Reusable

Worst Case

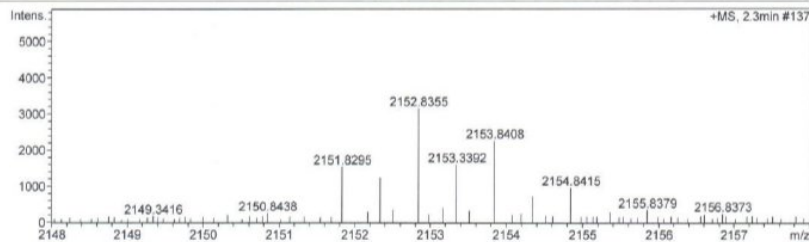


Mass Spectrum SmartFormula Report

Analysis Info
 Analysis Name D:\Data\SHUJVFENXI\yubiaogroup\2015110-7-76_RB5_01_20328.d
 Method 20150915.m
 Sample Name 2015110-7-76
 Comment
 Acquisition Date 5/13/2020 10:10:26 PM
 Operator BDAL@DE
 Instrument / Ser# maXis 4G 21240

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	220 °C
Scan Begin	300 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	2900 m/z	Set Collision Cell RF	2000.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
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2151.82892

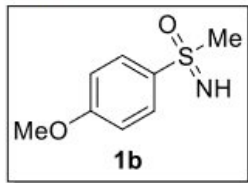
2152.831487

2151.8291⁻

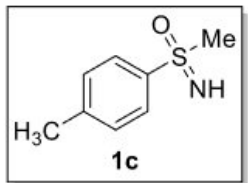
X. Shao, X. Wang, K. Zhu, Y. Dang, B. Yu,
J. Org. Chem. **2020**, 85, 12080-12096
 DOI: 10.1021/acs.joc.0c01191



Looking Neater, Still Worst Case



1-Methoxy-4-(S-methylsulfonimidoyl)benzene (1b). Isolated in 95% yield (907.1 mg, 4.90 mmol) as a faint yellow solid. ^1H NMR (600 MHz, $\text{DMSO}-d_6$) δ 7.85 (d, $J = 8.8$ Hz, 2H), 7.11 (d, $J = 8.8$ Hz, 2H), 4.05 (s, 1H), 3.84 (s, 3H), 3.02 (s, 3H). ^{13}C NMR (151 MHz, $\text{DMSO}-d_6$) δ 162.3, 135.7, 129.4, 114.1, 55.6, 46.3.



1-Methyl-4-(S-methylsulfonimidoyl)benzene (1c). Isolated in 72% yield (608.4 mg, 3.60 mmol) as a faint yellow oil. ^1H NMR (600 MHz, $\text{DMSO}-d_6$) δ 7.81 (d, $J = 8.0$ Hz, 2H), 7.40 (d, $J = 7.6$ Hz, 2H), 4.12 (s, 1H), 3.03 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (151 MHz, $\text{DMSO}-d_6$) δ 143.2, 141.7, 129.9, 127.8, 46.3, 21.4.

Assigned

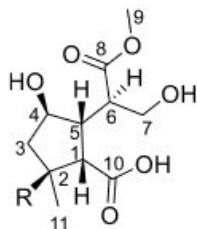
x

Machine-readable

x

S. Li, L. Liu, R. Wang, Y. Yang, J. Li, and J. Wie,
Org. Lett. **2020**, 22, 7470-7474
DOI: 10.1021/acs.orglett.0c02615

Slightly Better



1: R = OH
2: R = OAc

Journal of Natural Products

Table 1. ^1H , ^{13}C , and HMBC NMR Spectroscopic Data for **1** (800 MHz, Methanol- d_4)

position	δ_{C} , type	δ_{H} , m (J in Hz)	HMBC, H \rightarrow C
1	61.9, CH	2.78, dd (6.8, 1.9)	C-1, C-2, C-3, C-4, C-5, C-10
2	79.9, C-O		
3	49.6, CH ₂	2.42, dd (14.6, 9.6) 1.72, ddd (14.6, 2.5, 1.9)	C-2, C-4, C-5, C-11 C-1, C-2, C-4, C-5
4	76.7, HC-OH	4.40, ddd (9.6, 7.3, 2.5)	C-2, C-3, C-5, C-6
5	50.2, CH	2.70, ddd (11.4, 7.3, 6.8)	C-1, C-3, C-4, C-6, C-7, C-8
6	51.0, CH	2.87, ddd (11.4, 8.2, 4.9)	C-1, C-4, C-5, C-7, C-8
7	63.9, H ₂ C-OH	3.99, dd (11.2, 4.9) 3.85, dd (11.2, 8.2)	C-5, C-6, C-8 C-5, C-6, C-8
8	175.9, OC=O		
9	51.9, OCH ₃	3.69, s	C-8
10	175.8, COOH		
11	25.5, CH ₃	1.29, s	C-1, C-2, C-3

Assigned

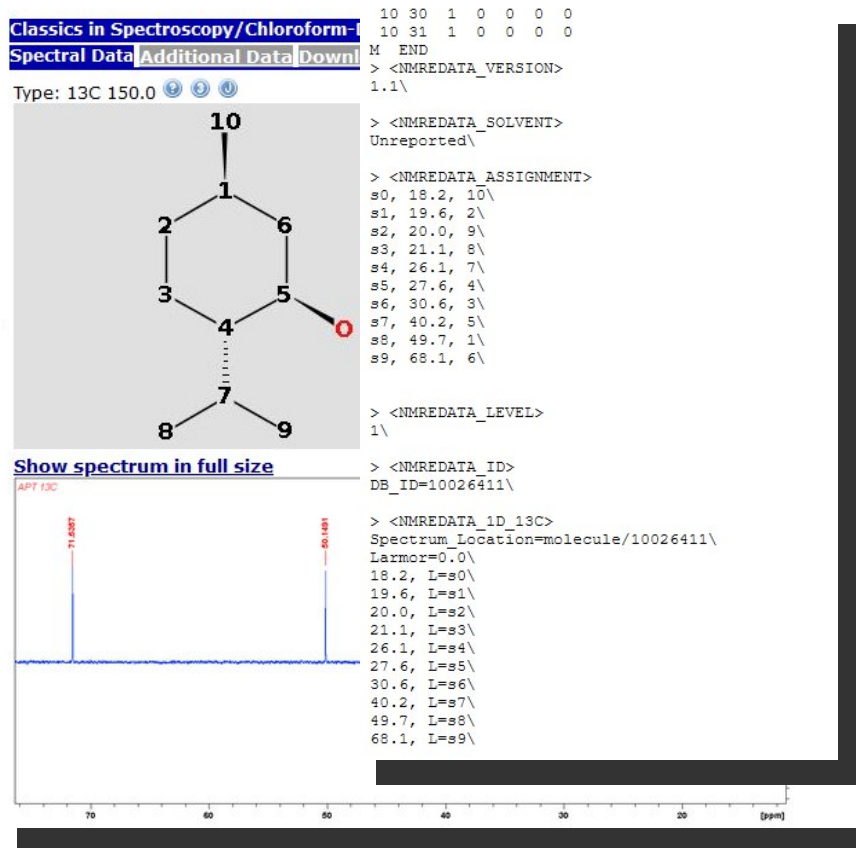


Machine-readable



L. Zandi, M. Makungu, J. J. E. Munissi, S. Duffy, R. Puttreddy, D. von der Heiden, K. Rissanen, V. M. Avery, S. S. Nyandoro, M. Erdélyi, *J. Nat. Prod.* **2020**, 83, 2641–2646.
DOI: 10.1021/acs.jnatprod.0c00447

First Steps in a Good Direction



Atom no. #	Mult.(coupling const.)	Meas. Shift
	D	31.6
	T	34.6
	T	23.2
	D	50.2
	D	71.5
	T	45.1
	D	25.8
	Q	21.0
	Q	16.1
	Q	22.2

Assigned
Machine-readable

Findable

Accessible

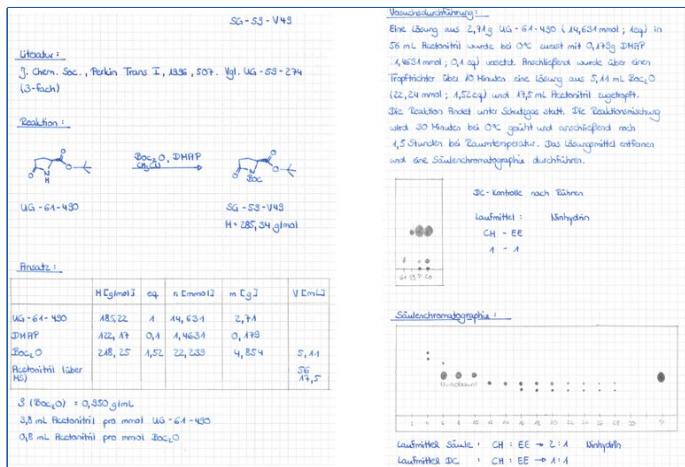
Interoperable

Reusable

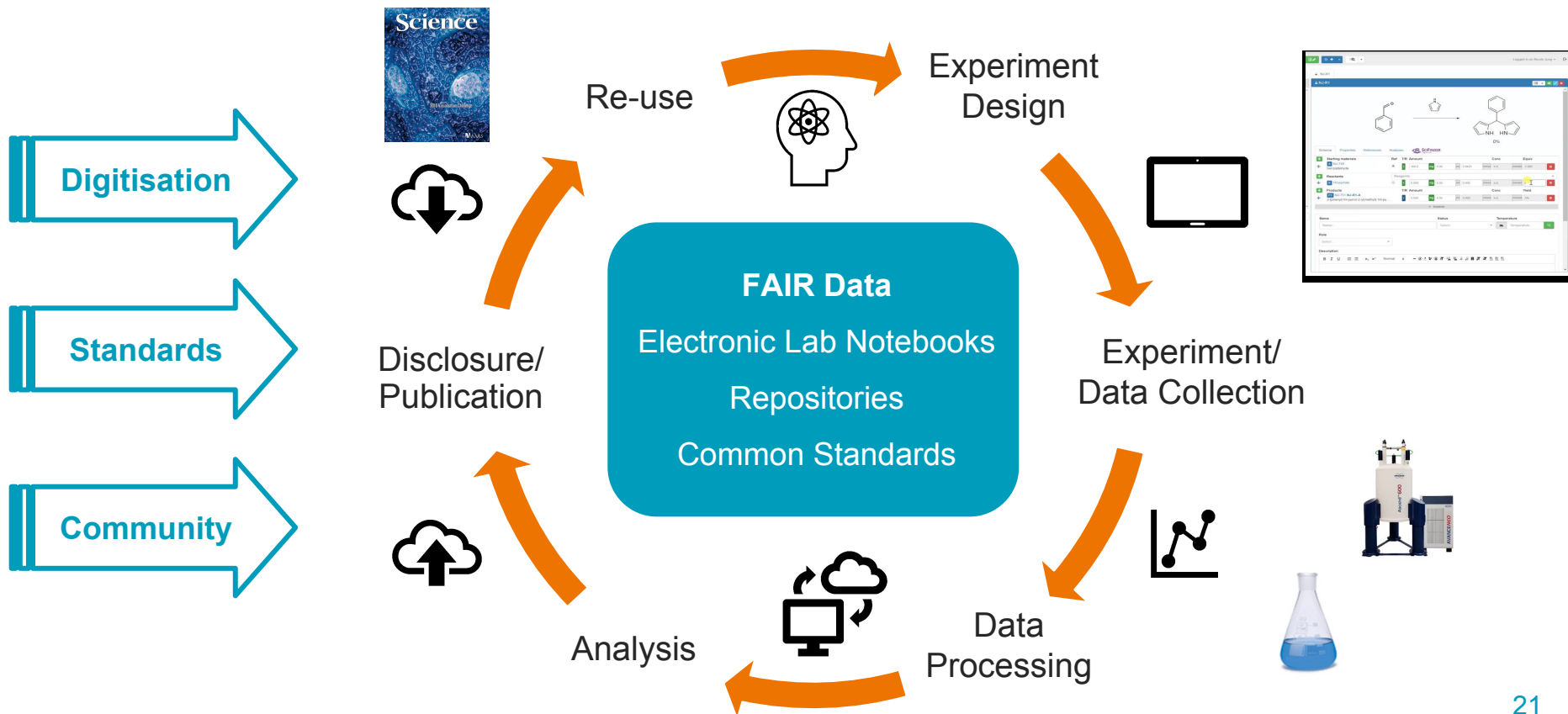
= FAIR

<https://www.nmrshiftdb.org>

Entry 10026411



Our Vision



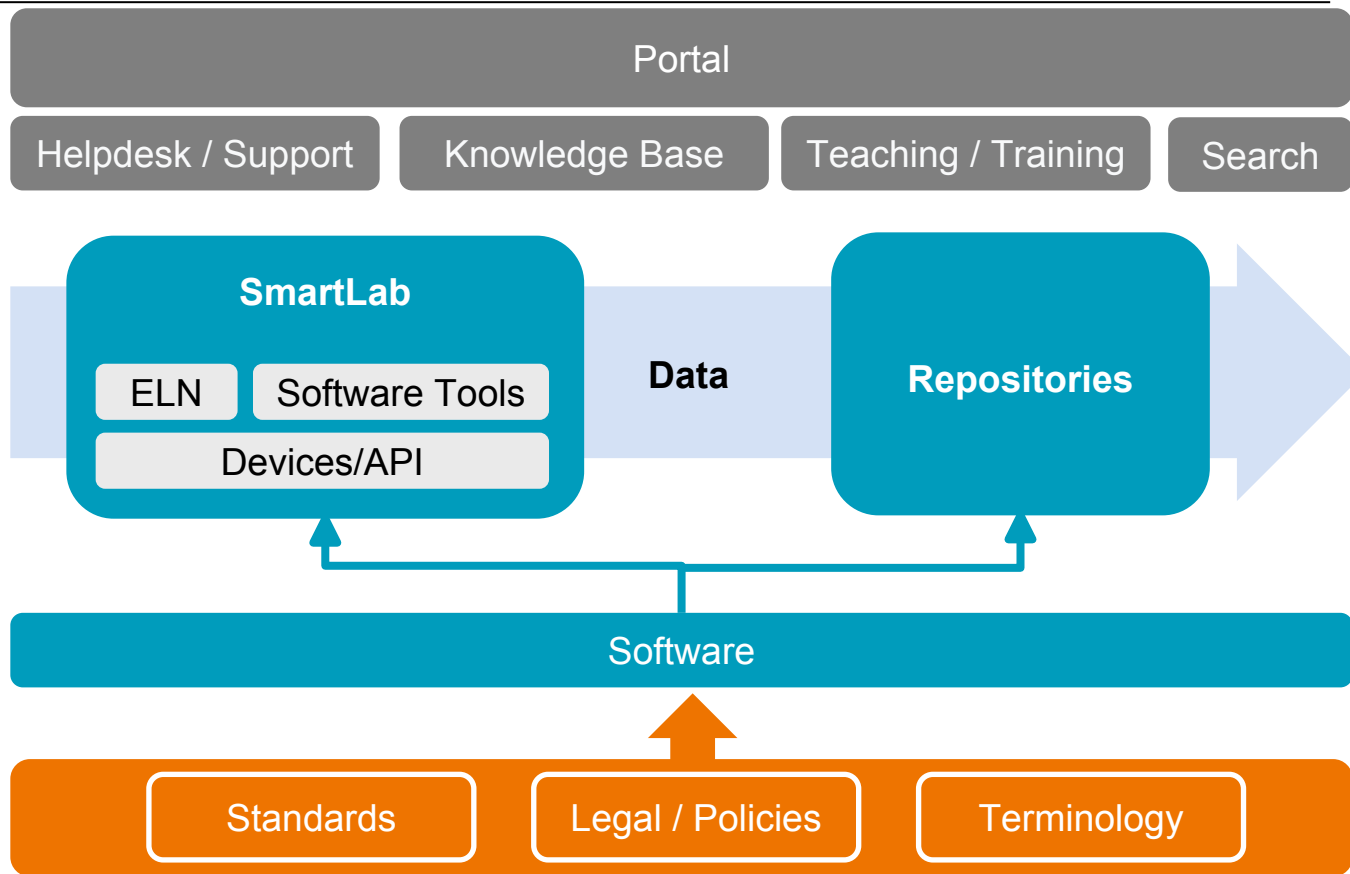


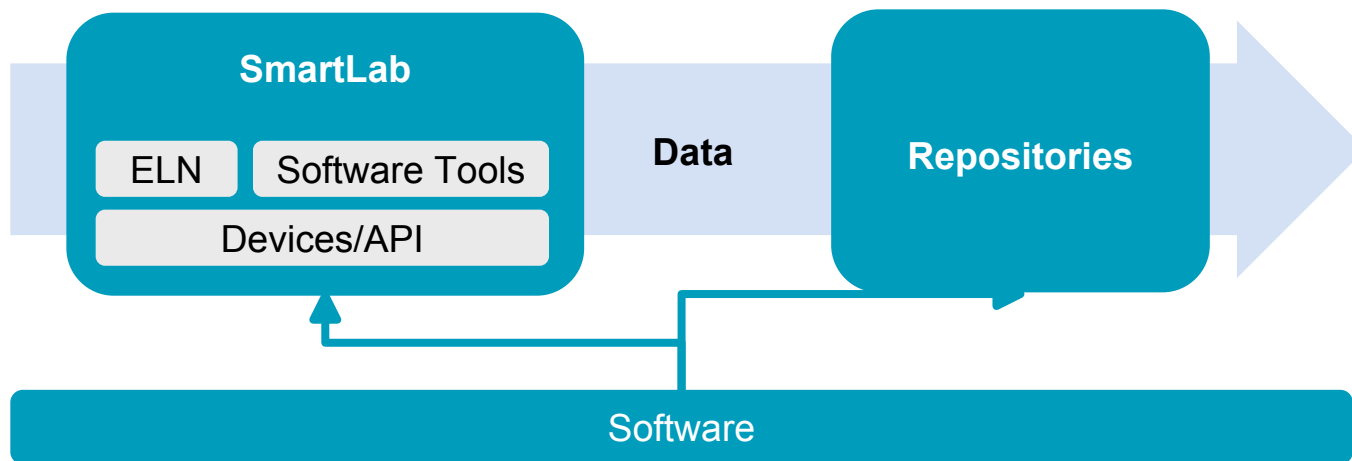
NFDI₄Chem

ENHANCE
YOUR
DATA.

What is our Strategy?

Strategy





Smart Lab - Seamless Data Flows

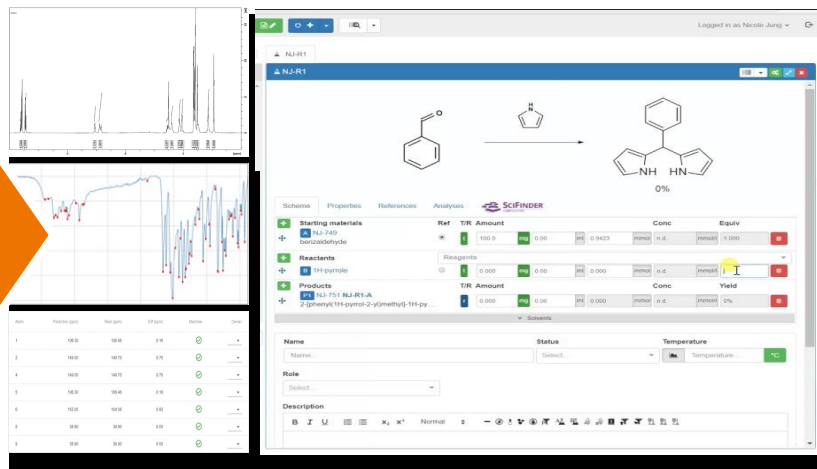


Devices



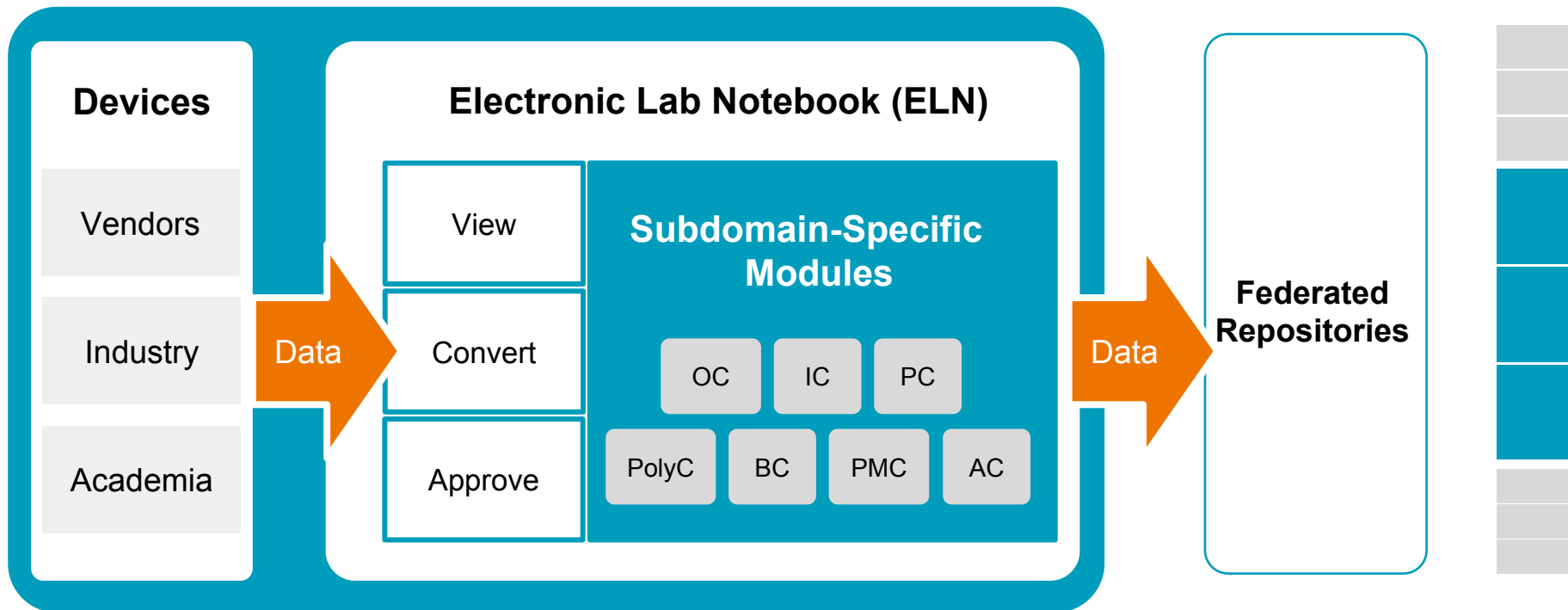
Data

Electronic Lab Notebook (ELN)

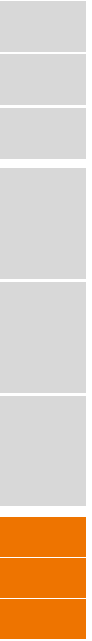


Federated
Repositories

Smart Lab - Seamless Data Flows

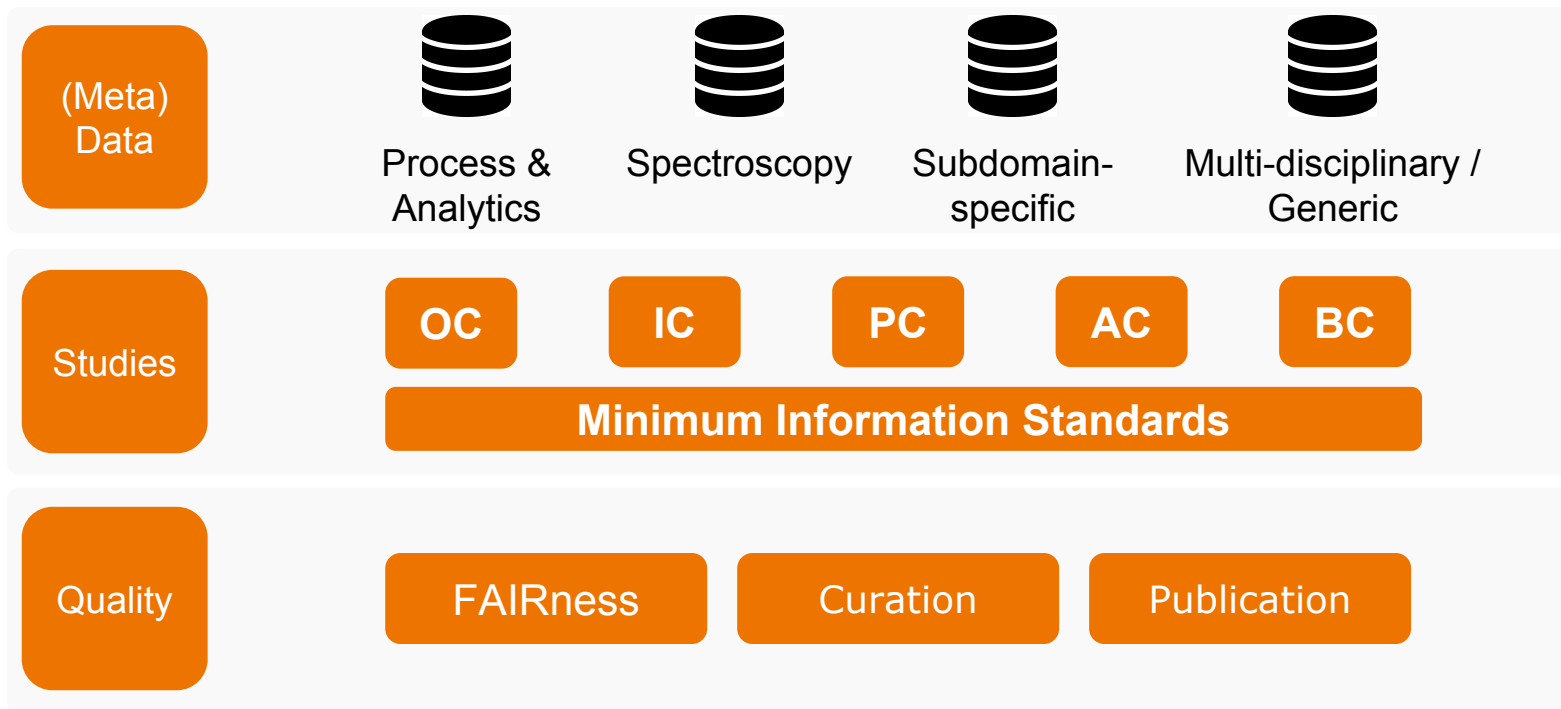


Standards



Standards

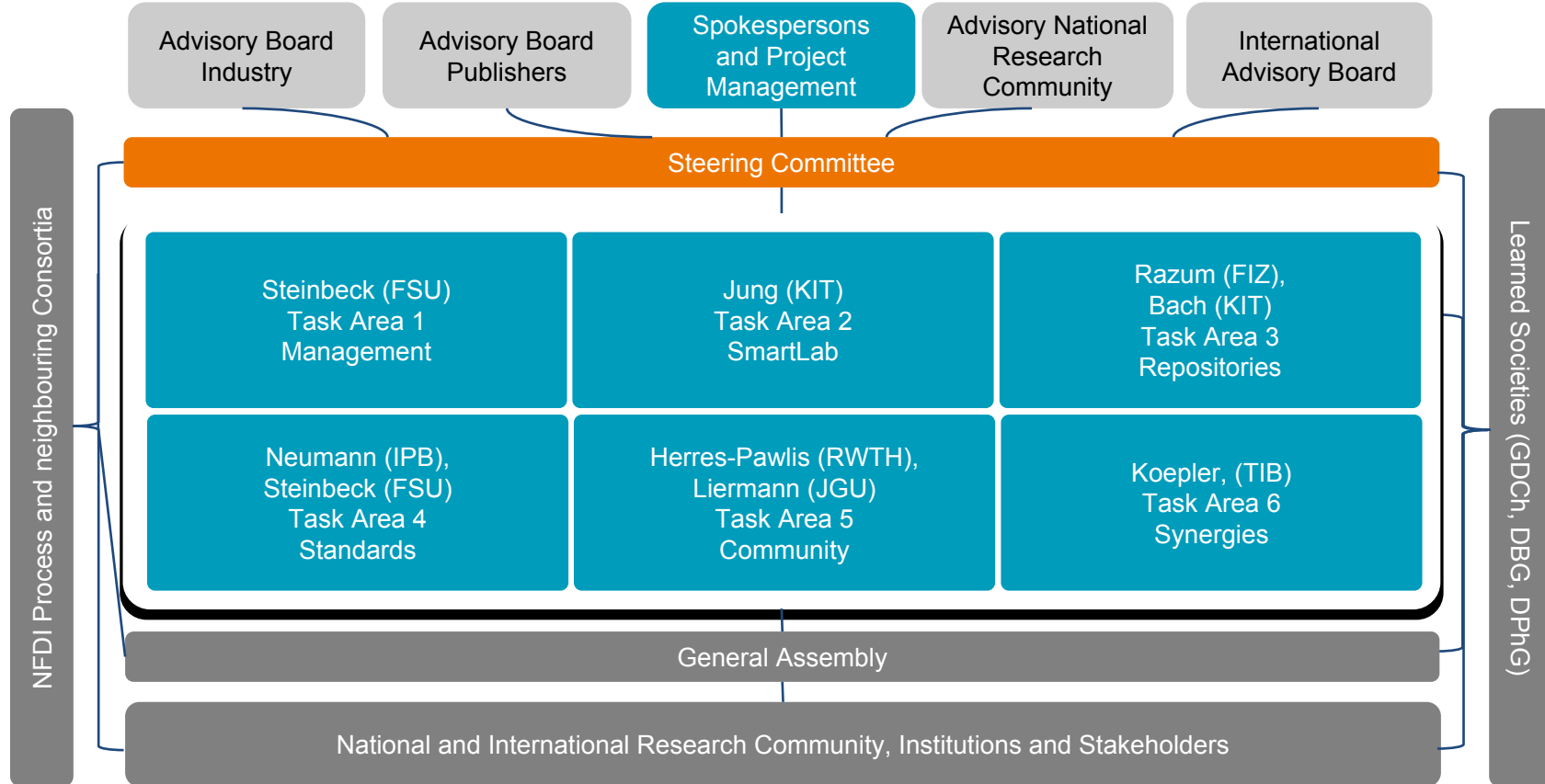
Standards



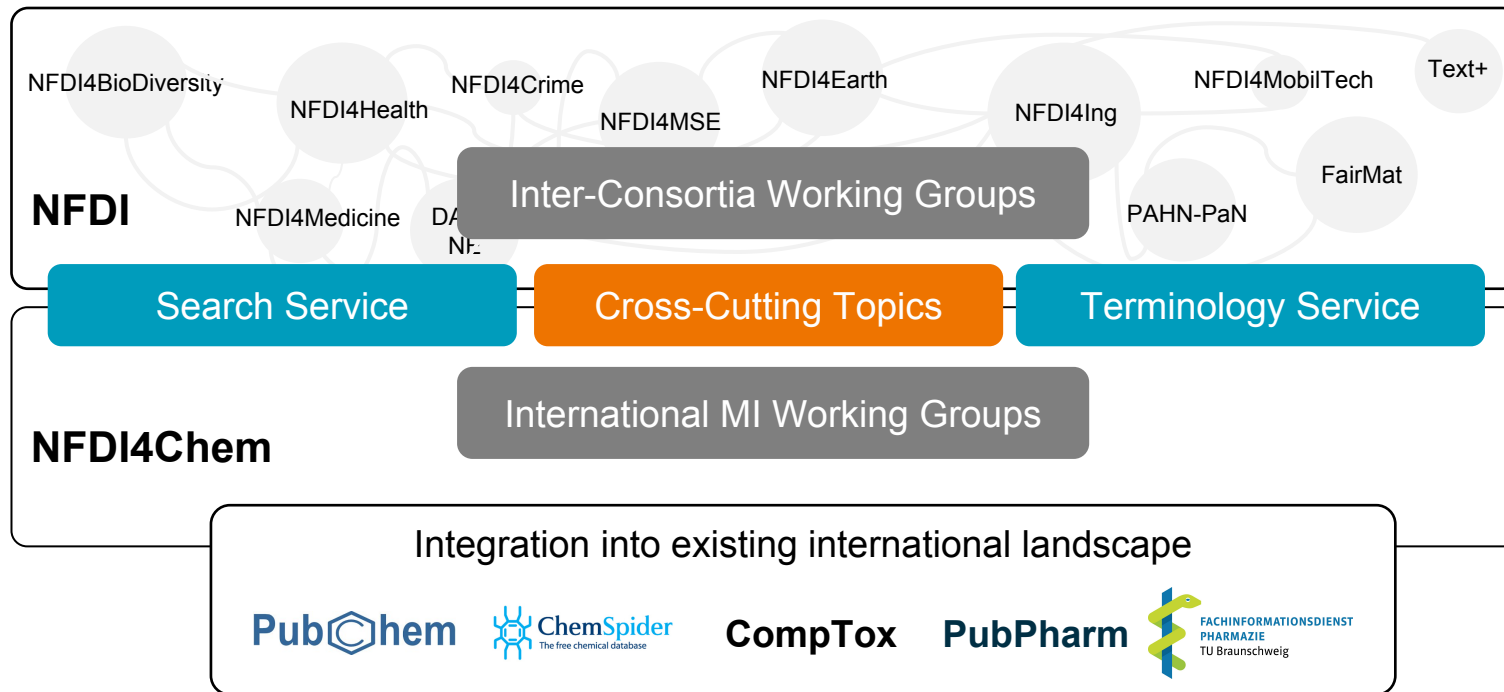
International Community Processes supported by NFDI4Chem



The Overall Picture



Synergies - Cross Cutting Topics



Involvement of the Community



Community requirements



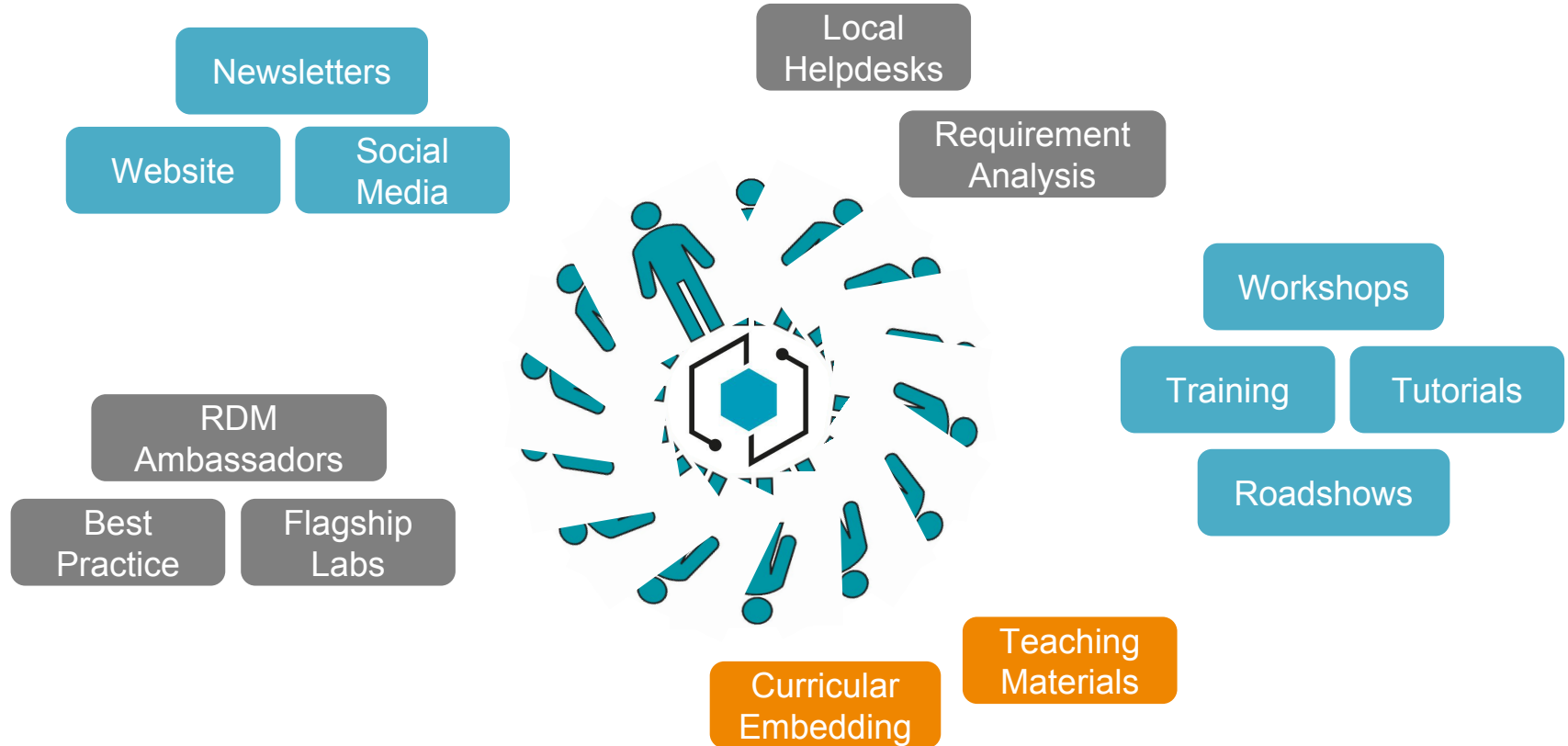
Fostering cultural change

Raising RDM awareness

RDM
Infrastructure



Involvement of the Community



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 (such as DFG) to determine FAIR requirements to fund research



VS.



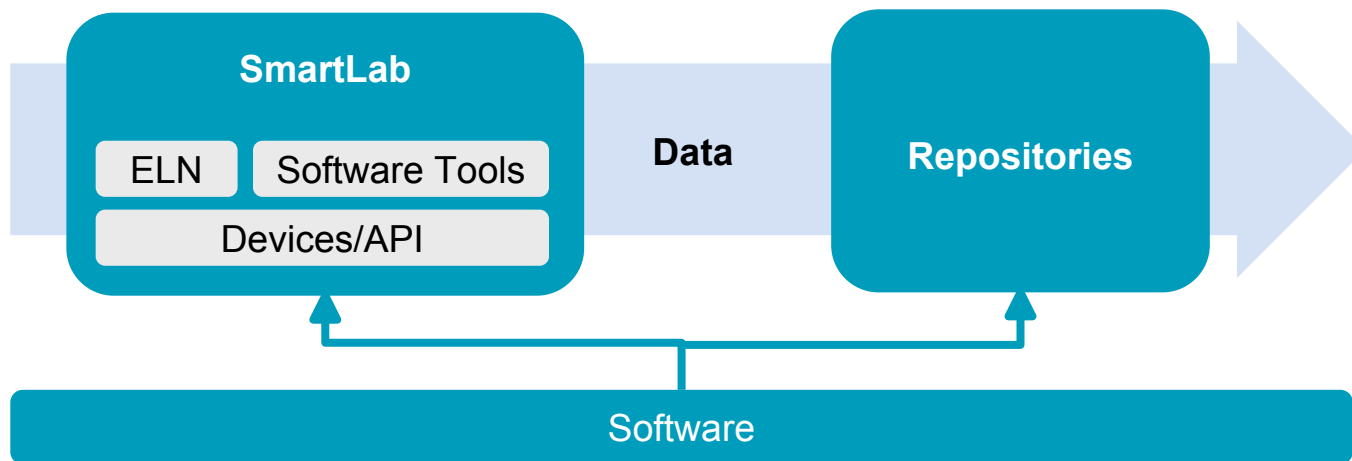


NFDI₄Chem

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DATA.

What do we offer?

ELNs & Repositories



Advantages of an ELN



Avoid Data Loss

- Linking experimental descriptions to collected data (analog and digital)
- Secure data storage



F
Findable



A
Accessible



I
Interoperable



R
Reusable

Standardised Documentation

- Structured and standardised collection of metadata
- Generation of interoperable (meta)data

Knowledge Management

- Data are findable
- Data are accessible
- Data are available, even after change of personnel!

Publication

- Data provision for publication of research results
- Simple transfer of data to repositories

A plethora of available ELNs



scif^ormation



What are the costs?

Where is the data hosted (cloud, local server)?

How is it accessed (web-based, local)?

How are the data secured?

Who is the technical maintainer of the ELN?

Does the ELN cover all my (sub)disciplines requirements?



SciNote

... any many more



A plethora of available ELNs

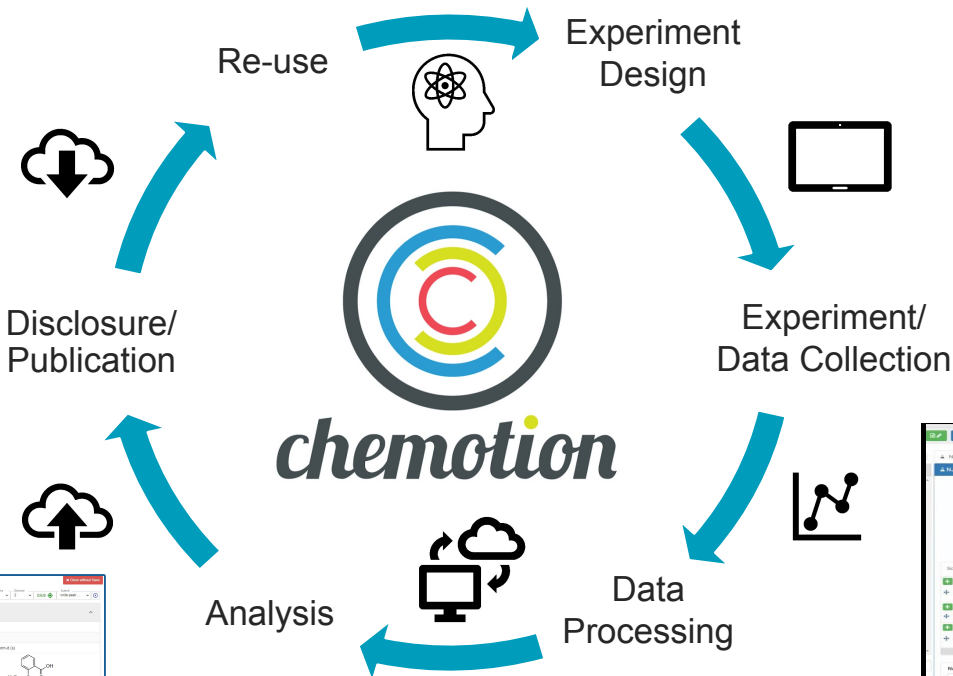


Chemotion – ELN & Repository



Chemotion-Repository Publikations Newsroom 11 How To 10

ID	Embargo	Author	Analyses	X-Total
CRR-19983		Juliane Klein	Analyses 6	X-Total
CRR-19980		Christoph Zippel	Analyses 4	X-Total
CRR-17667		Christoph Zippel	Analyses 4	X-Total



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

Start: [] Stop: [] Duration: [] Input Duration: []

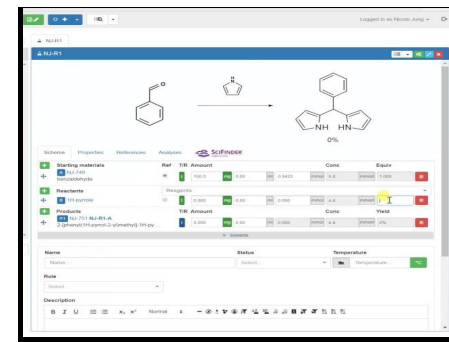
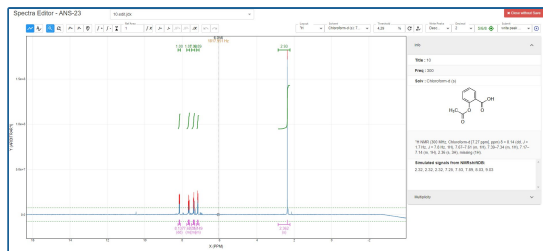
Type (phase Reaction Ontology): [] Role: []

Description: []

Purification: []

Purification Solvents	TR Label	Vol	Vol ratio
Water	Water	30.0	1.0
1,4-Dioxane	1,4-Dioxane	30.0	1.0

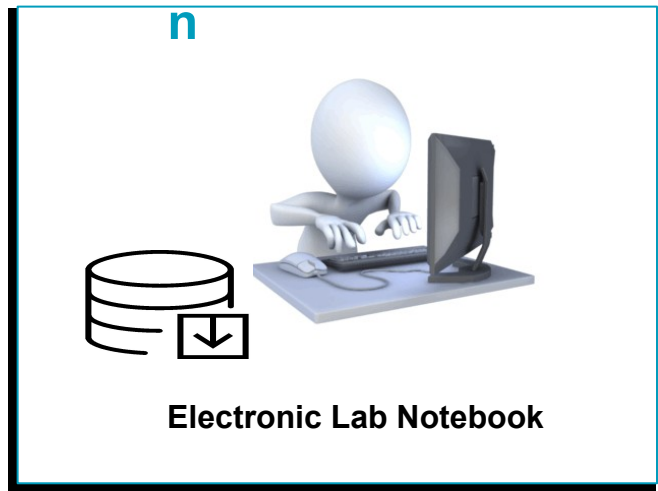
Additional information for publication and purification details



The challenge: Digitalization

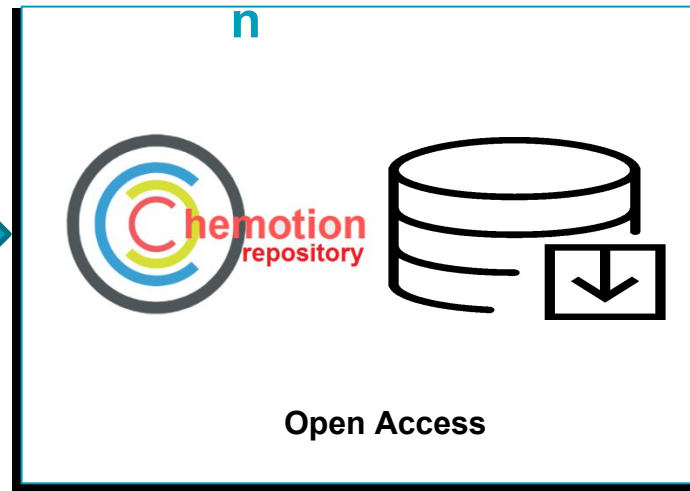


Documentation



select data & transfer

Publication

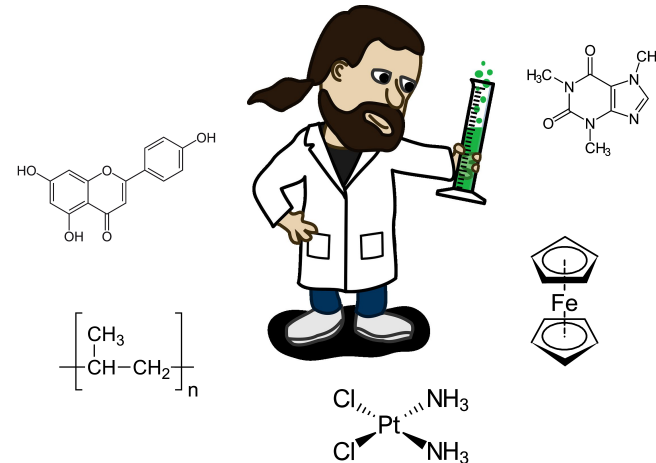


A few clicks to Open Data

Chemotion – an Open Source ELN



- Developed by Karlsruhe Institute for Technology in collaboration with NFDI4Chem partners
- ELN for Chemistry (and related disciplines)
- Advantages:
 - Browser-based (Chrome)
 - Drawing of chemical structures
 - Creation, description and documentation of reactions
 - Analysis of spectra & characterisation of samples
 - User management: access rights, sharing & syncing
 - Link to Chemotion repository



Basic view



Chemotion - All - IUPAC, InChI, SMILES, RInI

Collections: 128(0) 1751(0) 3(0) 11(0)

All

- chemotion-repository.net
- Test Collection Data
- Lamella Example
- MOF Test collection
- SurfMoF Test Collection
- MOF examples
- Polymers
- Linker
- Metal-Precursor
- Calculation Doptants
- MOF collection
- Info_Exchange IFG_IBCS_IOC
- Extracted data
- Calculation OLED
- Calculation TADF
- Lamella Test Collection
- New Collection
- My Data
- Joachim
- Fabian
- My shared collections
- Shared with me
- Synchronized with me
- Inbox 14

NJ-R1591

NJ-R1566

NJ-R1590

NJ-R1578

NJ-R1565

NJ-R1577

NJ-R1589

NJ-R1591

1.0

100 °C, 2.5 hr

Toluene

77%

Scheme Properties Literature Analyses

Starting materials

Ref	L/ST/RAmount	Conc	Equiv
NJ-2940	100.0 mg	0.6842 mmol	1.000

Reactants

Reagents	L/ST/RAmount	Conc	Yield
1H-quinoxalin-2-one	100.0 mg	0.6842 mmol	1.000
tetrabutylazanium.bro...	220.6 mg	0.6842 mmol	1.000
O10P4	194.3 mg	0.6842 mmol	1.000

Products

L/ST/RAmount	Conc	Yield
NJ-2943 NJ-R1591-...	0.5262 mmol	77%

Solvents

Conditions

Name

Status

Temperature

Start

Stop

Duration

2.5

1 hour(s)

Type (Name Reaction Ontology)

Role

Key Elements of the ELN



 114(0)

Samples

- Samples
- Properties of chemical compounds

 16(0)

Reactions

- Documentation
- Calculation
- Assigning of *Samples*

 3(0)

Wellplates

- 96 Well-plate
- Design and description
- Assigning of *Samples*

 3(0)

Screens

- Overview of (biological) Experiments
- Multiple *wellplates*

 1(0)

Research Plan

- Generic and flexible
- Text, Tables, Pictures, Reactions, ...

ELN – module for SEM-measurements



Chemotion(Testing) - All IUPAC, InChI, SMILES, RIn

(Testing Instance) Nicole Jung

NJ-W1 Workflow

NJ-W1 New Workflow-Test

NJ-W1

Properties Analyses Attachments

Workflow

New Workflow-Test

Basic sample (bsample)

Sample Material Dimensions details Next

Cutting(cutting) x

Cutting (cutting)

Input_sample output_sample instrument temperature humidity

cutting_wheel cutting_velocity cooling_agent feed Next

Embedding(embed...) x

Embedding (embedding)

Next

Polishing Parameters(polishing) x

Polishing Parameters (polishing)

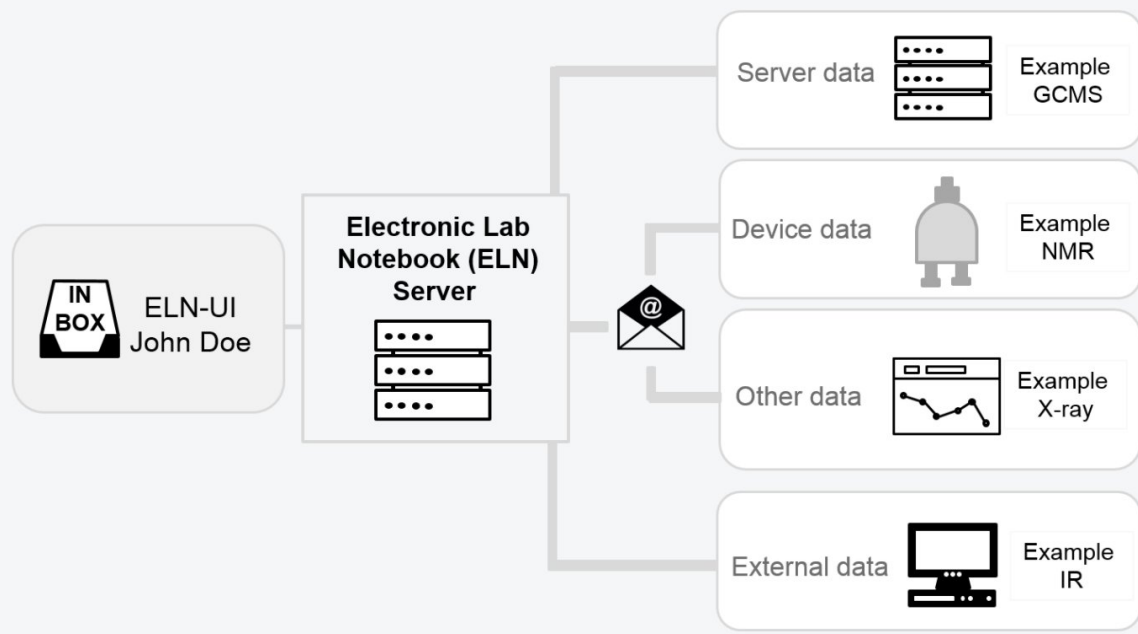
temperature humidity instrument Next

°C % Select...

Close Create

Nc1cc(Cl)ccc1Oc2ccccc2

Data transfer from devices to the ELN



Procedures for systematic capture and management of analytical data in academia

Jan Potthoff^a, Pierre Tremouilhac^b, Patrick Hodapp^b, Bernhard Neumair^a, Stefan Bräse^{a,c,*}, Nicole Jung^{a,c,*}

^a Institut für Organische Chemie, Karlsruhe Institute of Technology, Hermann von Helmholtz Platz 1, 76344 Eggenstein-Leopoldsdorf, Germany
^b Institute of Technology and Chemistry, Karlsruhe Institute of Technology, Hermann von Helmholtz Platz 1, 76344 Eggenstein-Leopoldsdorf, Germany
^c Institute of Organic Chemistry, Karlsruhe Institute of Technology, Fritz-Haber-Weg 6, 76173, Karlsruhe, Germany

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 Information and management systems
 Analytical data
 Infrastructure

ABSTRACT

Data management in universities is a challenging endeavor in particular due to the diverse infrastructure of devices and software in combination with limited budget. Nevertheless, in particular the analytical measurements and data sets need to be stored if possible digitally and in a well-organized manner. This manuscript describes how scientists can achieve a data management workflow focusing on data capture and storage by small adapters to commonly used systems. The presented workflow includes data transfer options from ubiquitous devices like NMR instruments, GC (MS) or LC (MS), IR and Raman, or mass spectrometers to a central server and the visualization of the available data files in an electronic lab notebook (ELN). The given instruments were chosen according to the needs of synthetic chemists, in particular devices needed in organic, inorganic and polymer chemistry where single data files in the range of several megabytes per data set are produced. Altogether, three different data transfer systems were elaborated to allow a flexible handling of different devices running with different proprietary software: The first procedure shows data capture via the use of a mail server as data exchange point. With the second procedure, data are automatically mirrored from a local file folder to a central storage server where new files are monitored and processed. The third procedure was designed to transfer data with manual support to a central server which is supervised to register new information. All components that are necessary to install and use the herein elaborated functions are available as Open Source and the designed workflow are described step by step to facilitate the adaptation of procedures in other universities accordingly if desired.
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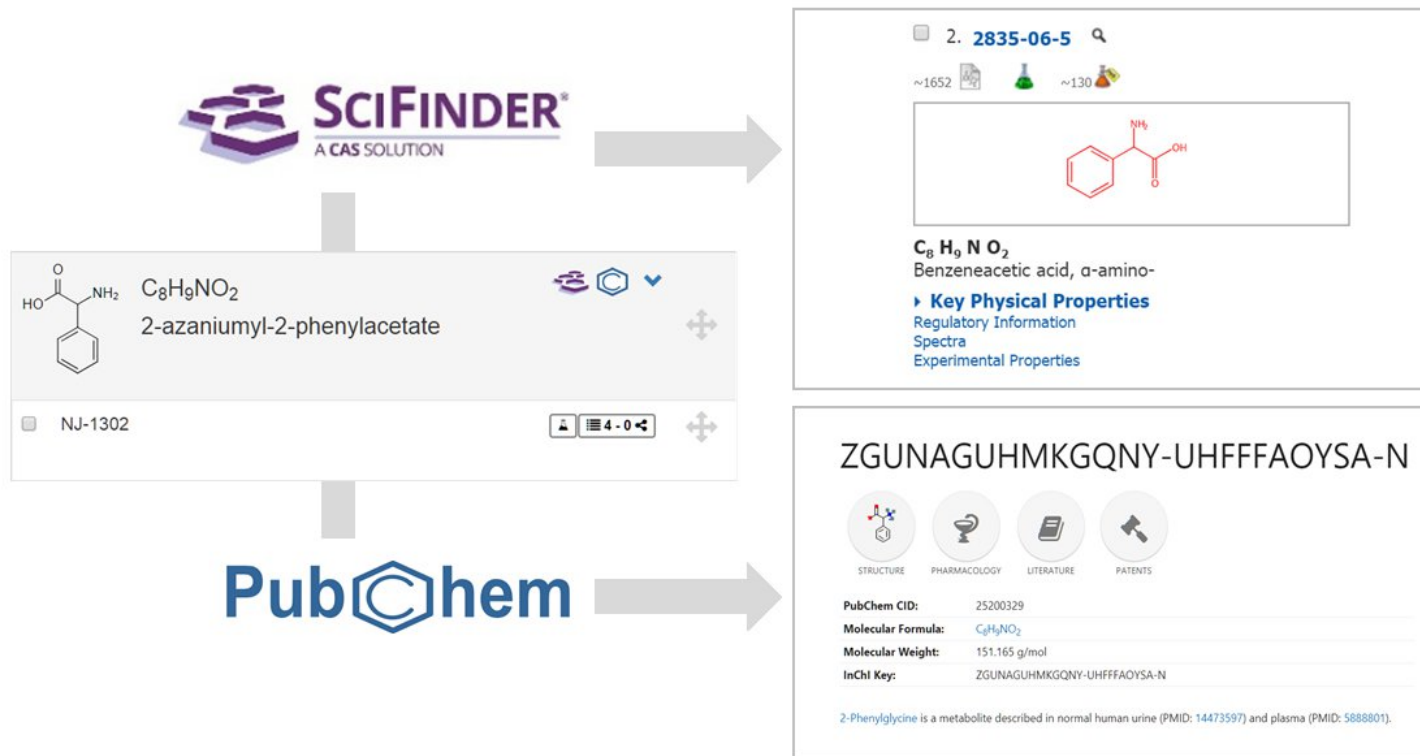
1. Introduction

Systematic data collection and management is of high importance in research institutions, in particular due to the increasing requirements to develop and meet research data management plans. Systems that support researchers in this area contribute to the improvement of the overall data structure and help scientists to keep the overview of analytical files. Additionally, management systems for analytical data allow the systematic storage of digital

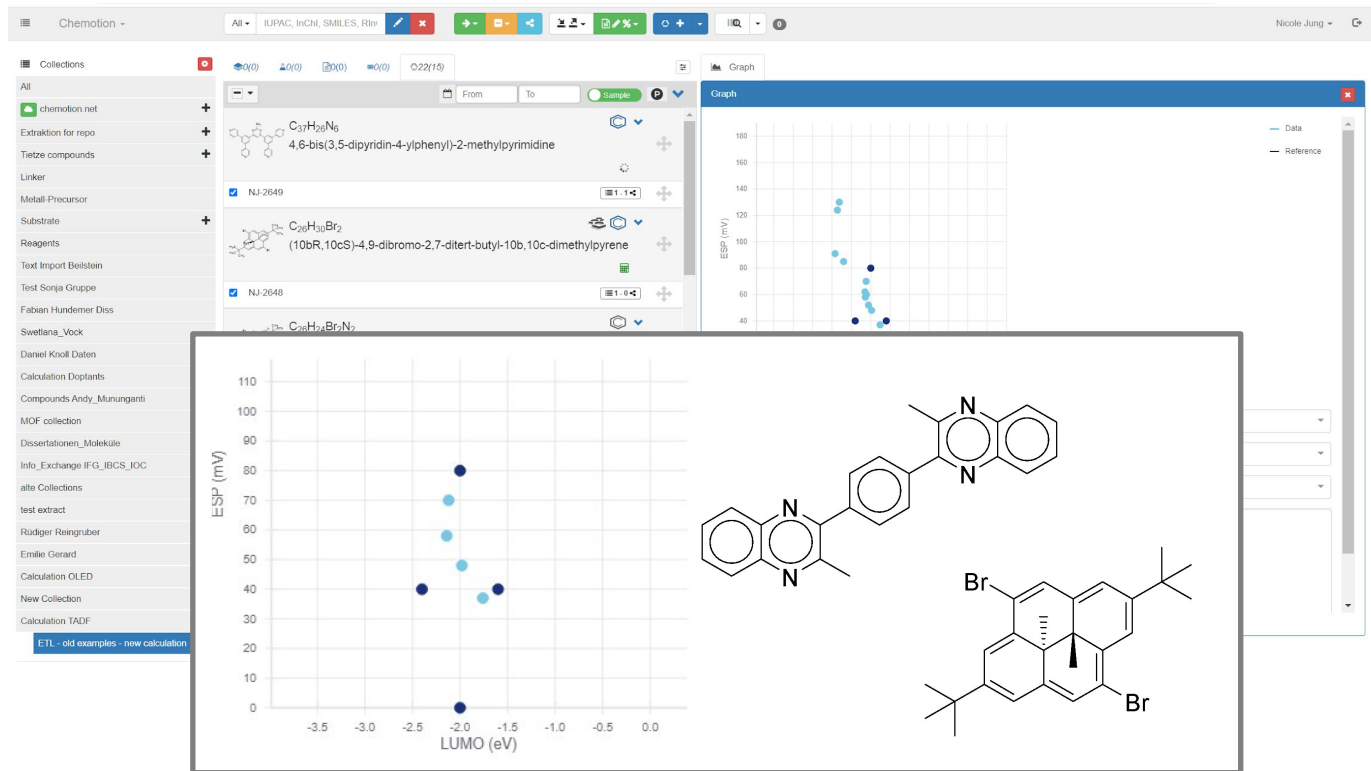
data which is of high importance e.g. for the accessibility of research data in compliance with the FAIR data [1] principles. In contrast to this need, the systematic capture and storage of analytical data in natural sciences and in experimental or analytical laboratories can be a challenging endeavor even for non-big data research due to the manifold sources of data and the use of different devices for their acquisition. Therefore, larger companies usually invest in Laboratory and Information Management Systems (LIMS) which allow to central the data workflow, data tracking, and data transfer. Some of the well-known systems are STARLIMS (Abbott Informatics Corporation) [2], Limsology (ABC Informa) [3], Biowis LIMS (Accelrys) [4], SampleManager (Thermo Fisher Scientific) [5], webLIMS (Labpro) [6] or LabInfo LIMS (Computing Solutions) [7]. A LIMS allows to reduce the errors that are inevitably associated with manual data handling. It prevents the loss of data, and improves the work efficiency, in particular with a high throughput of data. The

* Corresponding author. Institute of Organic Chemistry, Karlsruhe Institute of Technology, Fritz-Haber-Weg 6, 76173, Karlsruhe, Germany.
 E-mail addresses: stefan.braese@kit.edu (S. Bräse), nicole.jung@kit.edu (N. Jung).

ELN – connection to other databases



Simulation and calculation





NFDI₄Chem

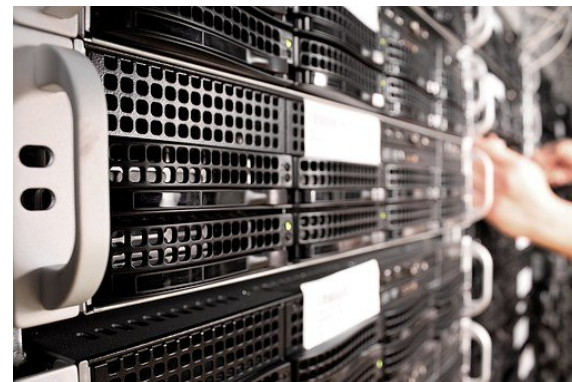
ENHANCE
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DATA.

How do I get Chemotion? How can I learn to use it?

Chemotion - first steps



- You can try out chemotion without any local installation via test-instances hosted at KIT
- Two options to run chemotion:
 - Local installation
 - NFDlin future: Chemotion as a service
- 4Chem provides technical support and training
- Interested? Contact helpdesk@nfdi4chem.de



Chemotion-ELN Handbook



- Comprehensive online manual
- Introductory videos
- In depth videos

The screenshot shows the 'Chemotion' online manual interface. The left sidebar contains a navigation menu with categories like 'Configuration', 'Manual', 'Introduction videos', 'Browser and access', 'Structure of the Chemotion ELN', 'Adjusting views', 'First steps', 'Collections', 'Lists in Chemotion ELN', 'Elements', 'Samples', 'Reactions', 'Wellplates', 'Details modal', 'Toolbar functions', 'Molecule editors/sketchers', and 'Barcodes and QR-codes'. The 'Samples' category is selected. The main content area is titled 'Samples in the element bar' and includes a paragraph explaining how samples are listed and represented in the interface, mentioning the benzene ring symbol and the number of samples within a collection.

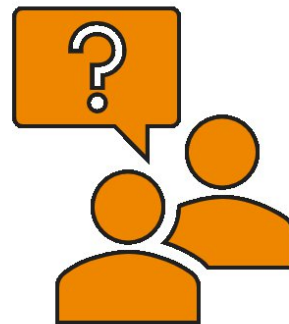
The screenshot shows the 'Chemotion' online manual interface, specifically the 'Introduction videos' section. The left sidebar is identical to the previous screenshot. The main content area is titled 'Introduction videos' and includes a paragraph explaining the purpose of the videos. Below the text are four video thumbnails arranged in a 2x2 grid, each with a play button icon. The thumbnails are labeled 'Part 1 Add collections', 'Part 2 Add reagents', 'Part 3 Plan a reaction 1', and 'Part 4 Plan a reaction 2'.

<https://chemotion.net/chemotionsaurus/docs/elN/intro>

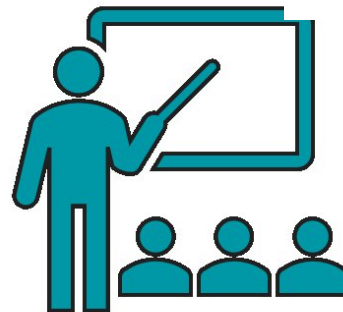
Chemotion-ELN Q&A Session



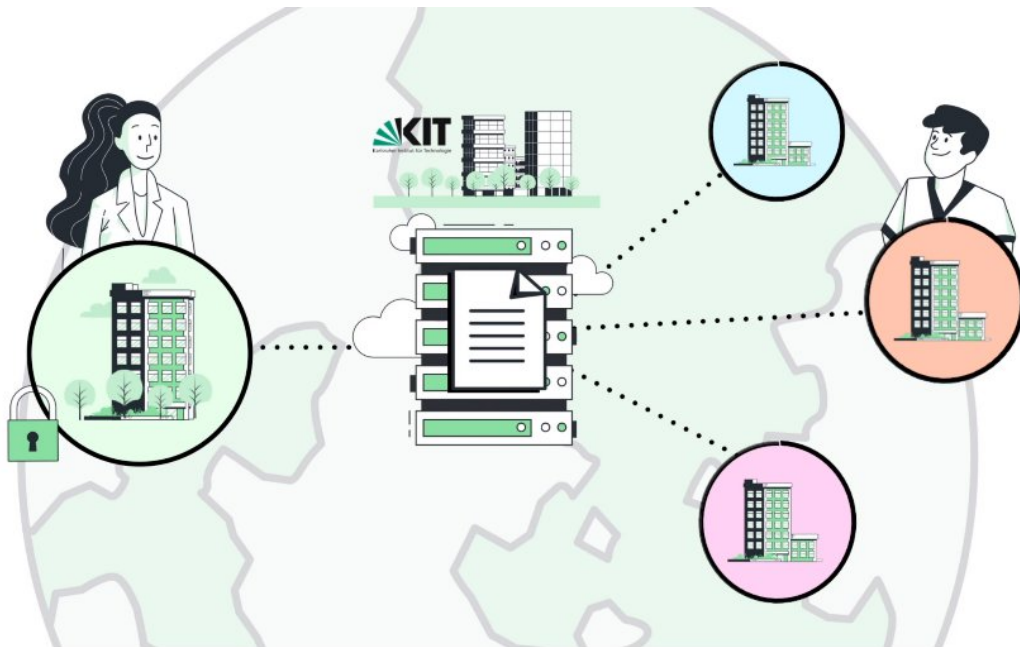
- Every second Thursday Chemotion Q&A
- Ask any questions or get help regarding Chemotion ELN
- General introductions to the ELN
- Next date:
 - Thursday, 27.01.2022, 15:00-16:00



Registration: via <https://www.nfdi4chem.de/>

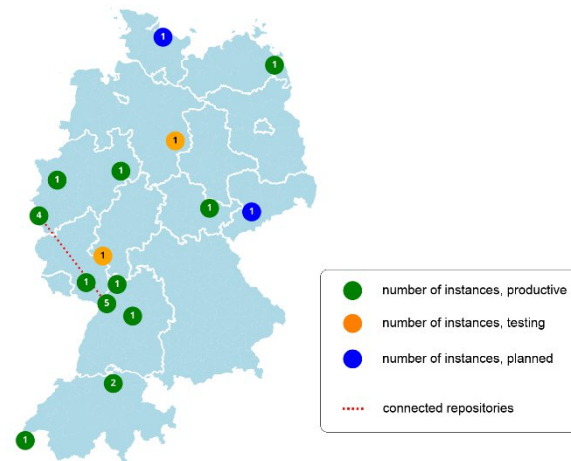


Infrastructure for the chemistry community



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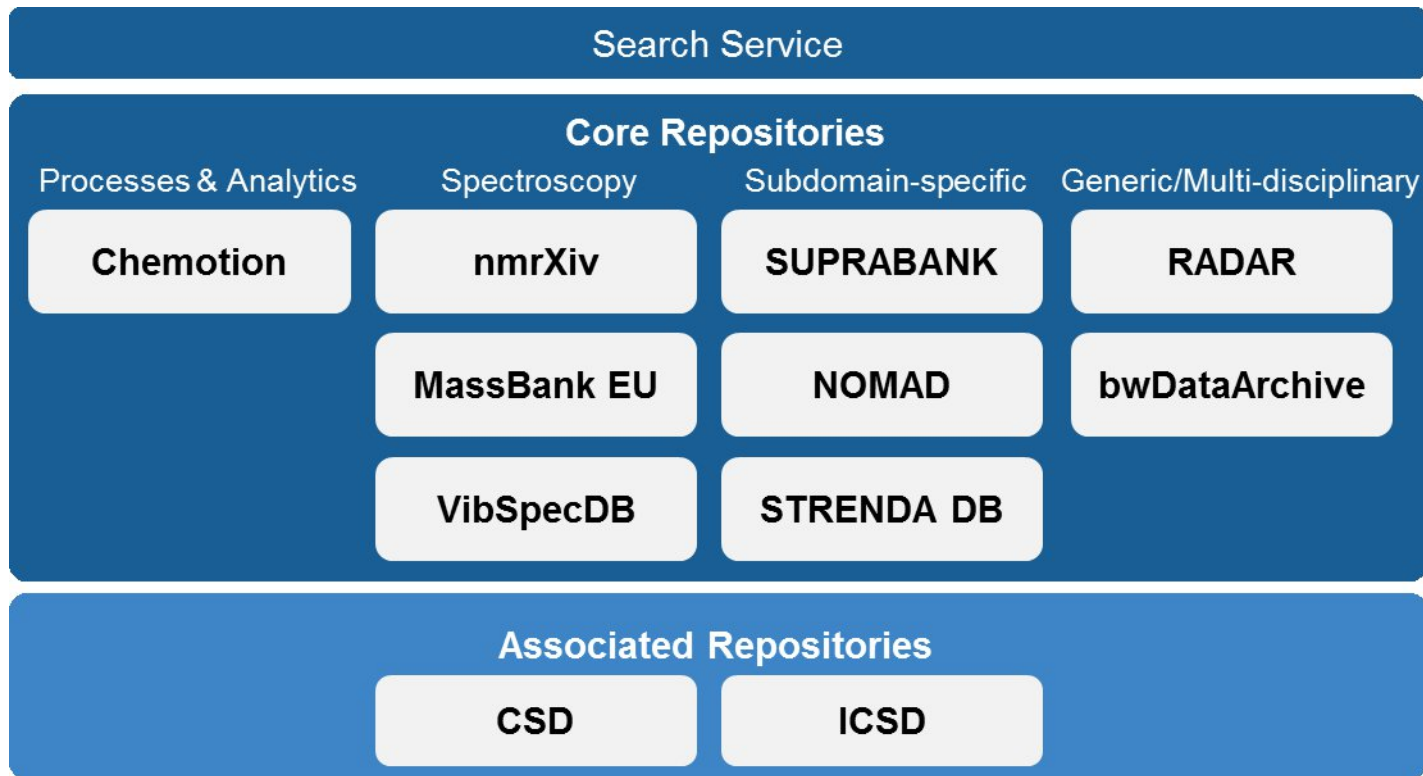


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Repositories in NFDI4Chem

Federation of repositories



The repository Chemotion



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nicole.jung@kit.edu

Published 3 days ago by Nicole Jung

Repository for molecules, reactions and research data

Visibility and Impact

- Publish your structures, attach your characterization data, and make them citable via DOI
- Automated registration at various scientific data providers
- Long-term archival - from scientists for scientists
- **NEW** Now, publish your Reactions

Samples

published
2531
556 under review
507 under embargo

Reactions

published
829
682 under review
493 under embargo

Analyses

published
7822
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2101 IR
1580 Mass

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Tie Digital Object Identifier (DOI) to your research data. This registers your data in DataCite and makes it identifiable, searchable and citable.

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Choose which license is suitable for your research data to allow others to re-use your data.

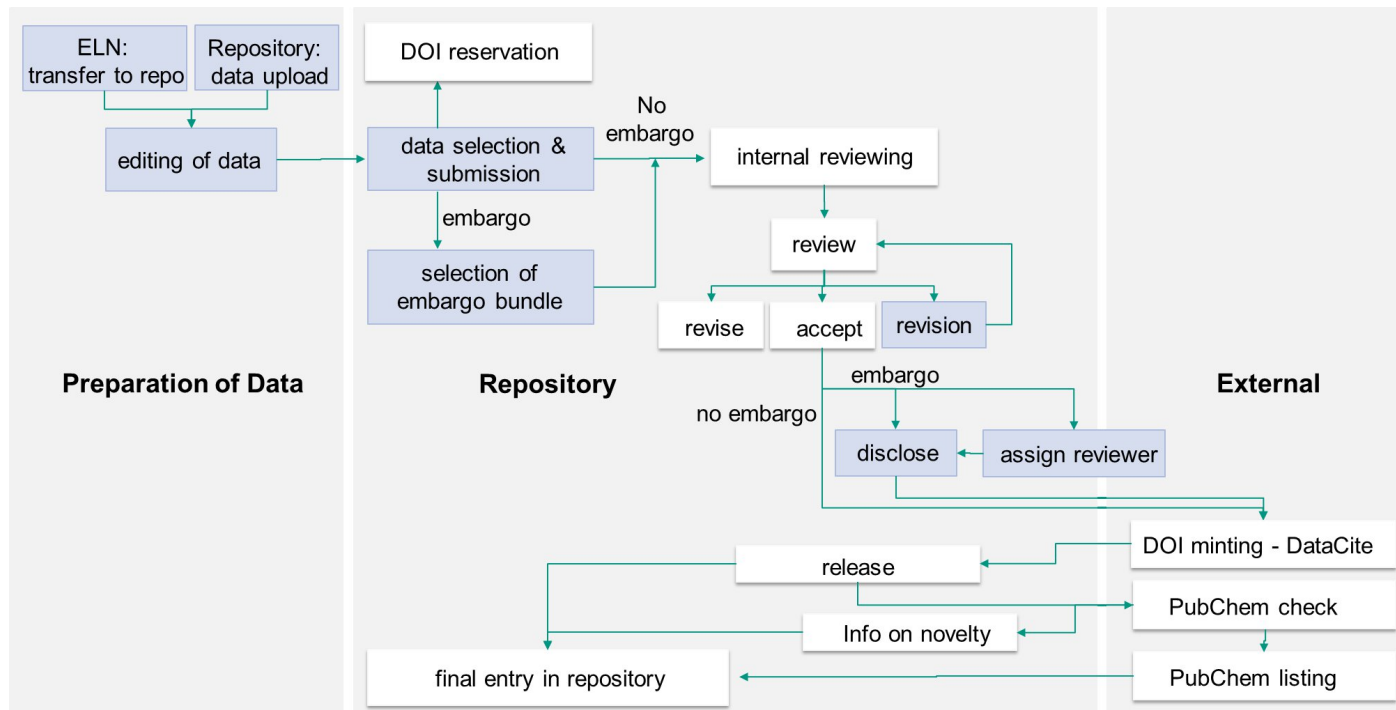
Data Quality

Release your research data and pass an internal review that ensures data quality.

Embargo

Put an embargo on your data. This allows you to delay the publication of your research data. You can release to make your research data visible to the public whenever you are

Workflow in chemotion repository



Reactions in chemotion repository



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Chemotion Initiative

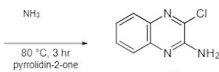


Q

Reactions

Samples

Scheme-only reactions



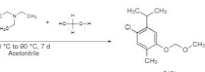
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Embargo

Author
Laura Holzhauser

Analyses
4

X-Vial
8



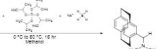
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Author
Simone Graßle

Analyses
8

X-Vial
-



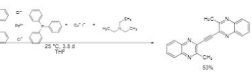
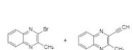
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Embargo

Author
Christoph Zippel

Analyses
4

X-Vial
-



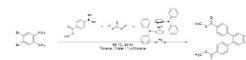
ID
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Author
Victor Larignon

Analyses
6

X-Vial
8



ID
CRR-19983

Embargo

Author
Jérôme Klein

Analyses
8

X-Vial
8



ID
CRR-19920

Embargo

Author
Christoph Zippel

Analyses
4

X-Vial
8



ID
CRR-17667

Embargo

Author
Christoph Zippel

Analyses
4

X-Vial
8



ID
CRR-17106

Embargo

Author
Victor Larignon

Analyses
6

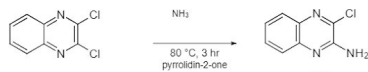
X-Vial
8

Reaction details in chemotion repository

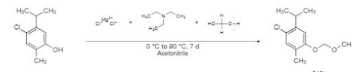


Chemotion-Repository My DB Publications Review Embargoed Publications

Q



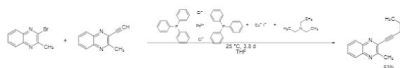
ID: CRR-20478 Embargo Author: Laura Holzhauser



ID: CRR-19765 Embargo Author: Simone Graßle



ID: CRR-19926 Embargo Author: Christoph Zippel



ID: CRR-19873 Embargo Author: Victor Larignon

¹H nuclear magnetic resonance spectroscopy (¹H NMR)

DOI: 10.14272/BMIMNRPAPYDN-UHFFFAOYSA-N/CHMO0000593



¹H NMR (400 MHz, DMSO-*d*₆, ppm) δ = 2.40 (s, 3H, CH₃), 7.23–7.28 (m, 2H, C₆H₄), 7.44–7.48 (m, 1H, C₆H₄), 7.67–7.69 (m, 1H, C₆H₄), 12.29 (s, 1H, NH).

Datasets

R53A_1H



¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)

DOI: 10.14272/BMIMNRPAPYDN-UHFFFAOYSA-N/CHMO0000595



¹³C NMR (400 MHz, DMSO-*d*₆, ppm) δ = 20.5 (1C, CH₃), 115.2 (1C, C₆H₄), 123.0 (1C, C₆H₄), 127.8 (1C, C₆H₄), 129.2 (1C, C₆H₄), 131.6 (1C, C₆H₄), 131.9 (1C, C₆H₄), 154.9 (1C, CNCH₃/CONH), 159.1 (1C, CNCH₃/CONH).

Datasets

R53A_13C



mass spectrometry (MS)

DOI: 10.14272/BMIMNRPAPYDN-UHFFFAOYSA-N/CHMO0000470



El (m/z, 70 eV, 100 °C): 161 (11) [M+H]⁺, 160 (94) [M]⁺, 132 (100), 131 (70).

Datasets

R53A_EI-MS



Infrared absorption spectroscopy (IR)

DOI: 10.14272/BMIMNRPAPYDN-UHFFFAOYSA-N/CHMO0000630



IR (ATR, $\bar{\nu}$) = 418, 453, 469, 476, 561, 584, 599, 691, 725, 751, 779, 853, 888, 928, 945, 1007, 1122, 1156, 1188, 1208, 1276, 1285, 1344, 1380, 1422, 1432, 1485, 1502, 1567, 1601, 1659, 2707, 2769, 2836, 2881, 2958, 3003, 3098 cm⁻¹.

Datasets

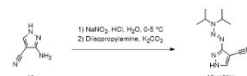
R53_IR



Generation of Supplemental Information



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



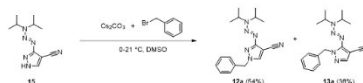
15: 5-[-(E)-[di(propan-2-ylamino)diazenyl]-1-[(H)-pyrazole-4-carbonitrile]. Formula: $C_{17}H_{26}N_{10}$. Exact Mass: 220.1436. Smiles: CC(C)N(C)C(C)N=Nc1c[nH]c2c1c[nH]c2C#N. InChIKey: UCFMQITXXMXHFF-CCEZHUSRSA-N

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 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 (bs, 1H), 7.76 (s, 1H), 5.27 (hept, J = 6.80 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 (s, C), 79.7, 50.8 (s, C), 47.6 (s, C), 23.4 (s, C), 19.2 (s, C), 18.0 (s, C). EI (m/z, 70 eV, 80 °C): 220 (100 [%]), 135 (23), 134 (11), 120 (35), 108 (16), 108 (37), 100 (32), 86 (37), 84 (38), 70 (15), 69 (13), 65 (23), 58 (74), 52 (21). HRMS (Calcd): 220.1436. Found: 220.1438. IR (ATR, ν = 3111, 2911, 2891, 1616, 1591, 1571, 1551, 1494, 1484, 1466, 1455, 1441, 1419, 1391, 1375, 1363, 1313, 1272, 1271, 1238, 1211, 1164, 1112, 1103, 1078, 1076, 1026, 1026, 946, 936, 909, 884, 850, 815, 785, 785, 722, 710, 691, 666, 666, 630, 615, 615) cm^{-1} .

Additional information on the chemical synthesis is available via Chemotion repository:
<https://doi.org/10.14722/reaction-SA-FUHFF-UHFFADPSC-UCPQMOTXXMXHFFADPSC-NUHFF-NRHPV-NUHFF-ZZZZ>
Additional information on the analysis of the target compound is available via Chemotion repository:
<https://doi.org/10.14722/UCPQMOTXXMXHFF-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. Bromobenzene (117 mg, 80 μ mol, 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: $C_{27}H_{32}N_{10}$. Exact Mass: 310.1906. Smiles: N#CC1c[nH]1N=N(C(C)C)C(C)C#N. InChIKey: AONLLYWWGOMLR-XUTLUPISA-N

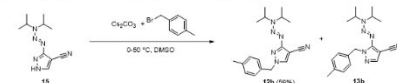
R_f = 0.23 (cyclohexane:ethyl acetate 4:1). 1H NMR (400 MHz, $CDCl_3$, ppm) δ = 7.53 (s, 1H), 7.30-7.15 (m, 5H), 5.32 (hept, J = 6.8 Hz, 1H), 5.13 (s, 2H), 3.93 (hept, J = 6.6 Hz, 1H), 1.15 (d, J = 6.8 Hz, 6H), 1.13 (d, J = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ = 162.9, 135.7 (s, C), 134.8, 129.1 (s, C), 128.8 (s, C), 128.3 (s, C), 128.3 (s, C), 115.3, 81.5, 56.9 (s, C), 49.9 (s, C), 46.5 (s, C), 23.3 (s, C), 19.3 (s, C), 19.3 (s, C), 18.0 (s, C), 18.0 (s, C). EI (m/z, 70 eV, 80 °C): 310 (100 [%]), 210 (60), 181 (13), 131 (17), 100 (48), 92 (13), 91 (100), 86 (10), 84 (14), 77 (22), 71 (12), 70 (10), 69 (35), 58 (54), 57 (23), 55 (53). HRMS (Calcd): 310.1906. Found: 310.1905. IR (ATR, ν) = 3122 (vs), 3058 (vs), 3031 (vs), 2979 (vs), 2934 (vs), 2868 (vs), 2223 (vs), 1816 (vs), 1700 (vs), 1604 (vs), 1537 (vs), 1497 (vs), 1456 (vs), 1412 (vs), 1368 (vs), 1355 (s), 1325 (vs), 1313 (vs), 1281 (vs), 1239 (vs), 1227 (vs), 1184 (vs), 1149 (vs), 1132 (vs), 1095 (vs), 1083 (vs), 1028 (s), 1001 (vs), 970 (vs), 949 (vs), 881 (vs), 831 (vs), 843 (vs), 819 (vs), 799 (vs), 752 (vs), 741 (s), 721 (vs), 711 (vs), 694 (s), 649 (vs), 632 (vs) cm^{-1} .

13a: (E)-1-benzyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-1H-pyrazole-4-carbonitrile. Formula: $C_{27}H_{32}N_{10}$. Exact Mass: 310.1906. Smiles: CC(C)N(C)C(C)N=Nc1c[nH]c2c1c[nH]c2C#N. InChIKey: AQYAXXLCHEFGV-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 = 158.4, 141.3, 115.4 (s, C), 79.7, 50.8 (s, C), 47.6 (s, C), 23.4 (s, C), 19.2 (s, C), 18.0 (s, C). EI (m/z, 70 eV, 80 °C): 310 (100 [%]), 210 (60), 181 (13), 131 (17), 100 (48), 92 (13), 91 (100), 86 (10), 84 (14), 77 (22), 71 (12), 70 (10), 69 (35), 58 (54), 57 (23), 55 (53). HRMS (Calcd): 310.1906. Found: 310.1905. IR (ATR, ν) = 3111 (vs), 3089 (vs), 3067 (vs), 3051 (vs), 2987 (vs), 2955 (vs), 2935 (vs), 2871 (vs), 2220 (s), 1761 (vs), 1606 (vs), 1537 (vs), 1494 (vs), 1466 (vs), 1455 (vs), 1441 (vs), 1419 (vs), 1391 (s), 1375 (vs), 1363 (vs), 1313 (vs), 1272 (s), 1238 (vs), 1211 (vs), 1164 (vs), 1112 (vs), 1103 (vs), 1078 (vs), 1026 (vs), 1026 (vs), 946 (vs), 936 (vs), 909 (vs), 884 (s), 850 (vs), 815 (vs), 785 (vs), 722 (vs), 710 (s), 691 (vs), 666 (vs), 630 (vs), 615 (vs) cm^{-1} .

Additional information on the chemical synthesis is available via Chemotion repository:
<https://doi.org/10.14722/reaction-SA-FUHFF-UHFFADPSC-KRANR5FKB-UHFFADPSC-NUHFF-NYGOA-NUHFF-ZZZZ>
Additional information on the analysis of the target compound is available via Chemotion repository:
<https://doi.org/10.14722/AONLLYWWGOMLR-XUTLUPISA-N.1>
<https://doi.org/10.14722/AQYAXXLCHEFGV-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-ylamino)diazenyl]-1-[(H)-pyrazole-4-carbonitrile] (15, 563 mg, 2.55 mmol, 1.00 equiv) was dissolved in 20 mL of DMSO. The solution was cooled to 0 °C. Cesium carbonate (1.08 g, 3.07 mmol, 1.20 equiv) and 4-bromobenzyl-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

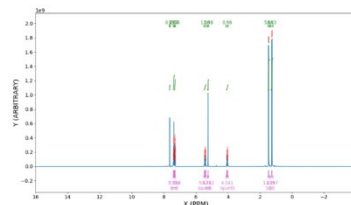
Synthesis of new pyrazolo[1,2,3]triazines by cyclative cleavage of pyrazolo-triazenes, Nicolai Wippert, Martin Nieger, Claudine Herlan, Nicole Jung and Stefan Bräse.
Beilstein Journal of Organic Chemistry, preprint 2021.

Generation of Supplemental Information

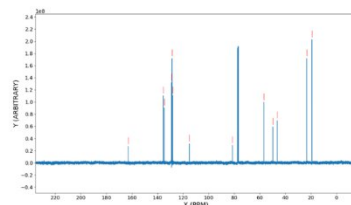


[12a] (E)-1-benzyl-3-(3,3-diisopropyltriaz-1-en-1-yl)-1H-pyrazole-4-carbonitrile

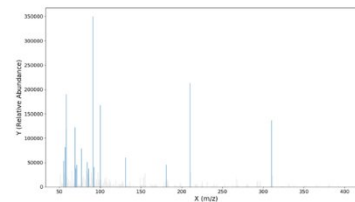
CHMO-0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



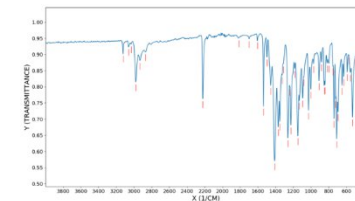
CHMO-0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO-0000470 | mass spectrometry (MS)



CHMO-0000630 | infrared absorption spectroscopy (IR)



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.



NFDI₄Chem

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DATA.

Further Services of NFDI4Chem



Portal

Helpdesk / Support





Helpdesk

Looking for information or help on research data management, data repositories or electronic lab notebooks (ELN) for chemistry?

Please check our [FAQ page](#) first. If you cannot find the information you are looking for, read on.

How to get in touch?

Contact our consortium-wide Helpdesk to get advice and support on most topics related to research data management, data repositories or electronic lab notebooks (ELN) for chemistry.

Either send an email to helpdesk@nfdi4chem.de or use the Helpdesk contact form below

Contact Helpdesk

What happens next?

Your request goes out to all members of the NFDI4Chem Helpdesk and will be picked up by the person with the greatest expertise on the particular topic.

Single point of entry to support you with all questions you may have regarding Research Data Management.

For example:

- Electronic Lab Notebooks (ELNs)
- Data Management Plans (DMPs)
- FAIR Data

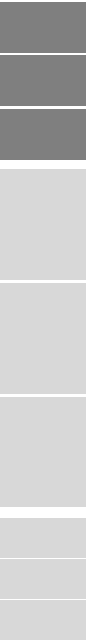
helpdesk@nfdi4chem.de

Knowledge Base



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Knowledge Base



NFDI4Chem Knowledge Base



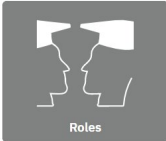
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NFDI4Chem Knowledge Base

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


[Get started](#)




Roles




Domains



Problems



Topics & Concepts

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- Launch in December!
- Linked to a Github repository
→ everyone can contribute
- Access to Research Data Management (RDM) knowledge via various points of entry
- Particular focus on chemistry-relevant topics such as data formats

Launch in December – watch this space

Teaching & Training



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Teaching / Training



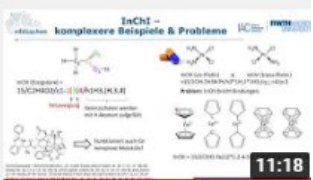








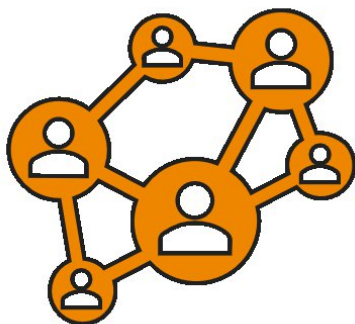
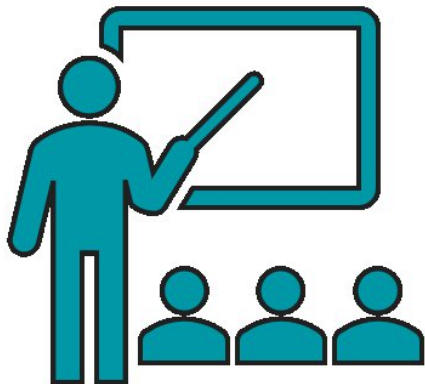
NFDI4Chem Youtube channel



- Introductory videos
- Recordings of talks and presentations

More videos in
pipeline for 2022 –
stay tuned!

 <p>9:58</p>	 <p>3:55</p>	 <p>11:18</p>
1. Stammtisch Chemotion (01/29/21) Overview of...	Ontologien - was ist das eigentlich?	FDM (5) - InChI & SMILES 55 views • 8 months ago
 <p>4:43</p>	 <p>4:27</p>	 <p>4:11</p>
FDM (4) - Metadaten	FDM (3) - Datenmanagementplan	FDM (2) - FAIR Prinzipien
 <p>10:05</p>	 <p>56:19</p>	 <p>45:22</p>
FDM (1) - Grundlagen 122 views • 8 months ago	NFDI4Chem Web Seminars - Joint Webinar Ontologies in...	NFDI4Chem Web Seminars - 01. General Concepts and...



- NFDI4Chem to give general talks about the consortium and RDM throughout the country
- NFDI4Chem Stammtisch last Friday every Month
- Chemotion introduction session every 2 weeks
- Hands on workshops coming soon:
 - Workshop: FAIR Research Data Management: Basics for Chemists
 - Chemotion ELN

Workshop: FAIR RDM: Basics for Chemists



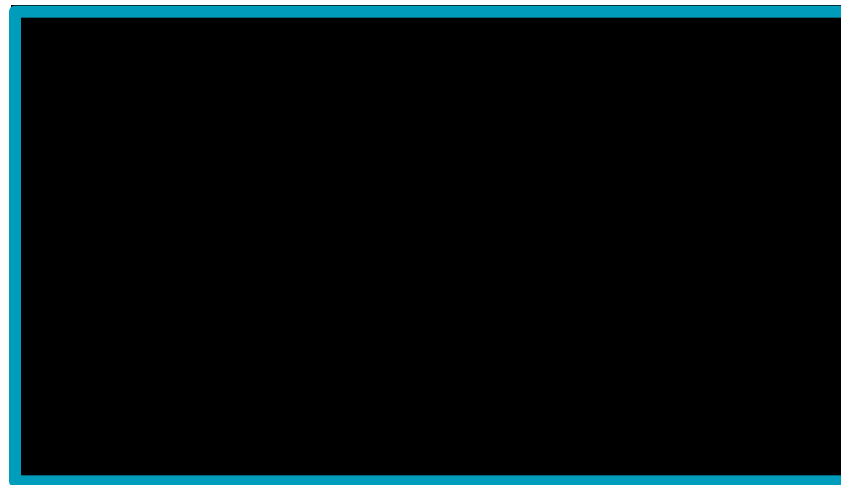
Costs: Free

Venue: Online

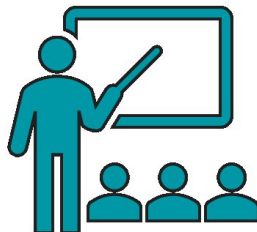
Duration: 2 days, 4-6 hours each

Participants: ~ 20 per Workshop

Registration: via <https://www.nfdi4chem.de/>



#	Day 1	Day 2
1	16.2.2022	18.2.2022
2	20.4.2022	22.4.2022
3	22.6.2022	24.6.2022
4	17.8.2022	19.8.2022
5	19.10.2022	21.10.2022
6	07.12.2022	09.12.2022



**Upon request, in-person
workshops at institutions**



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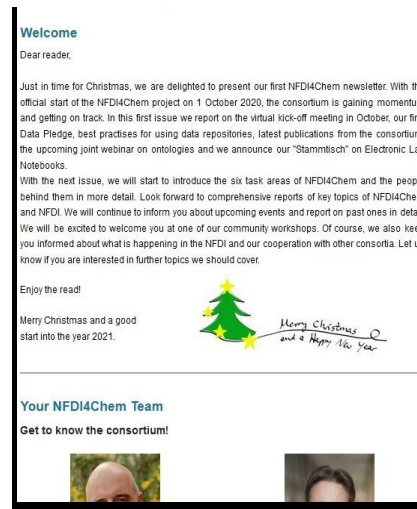
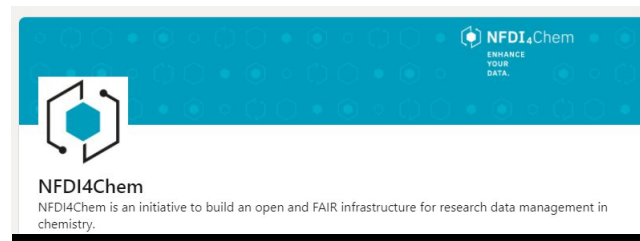
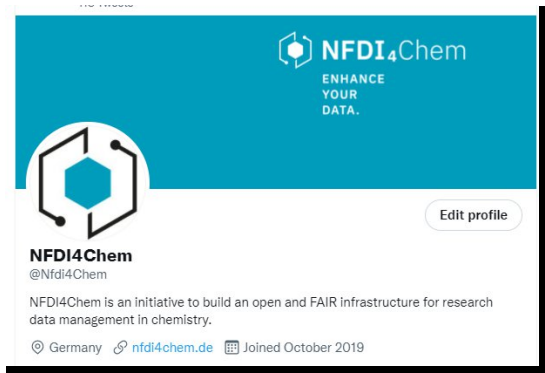


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Thank you for Listening! – Any Questions?