



DATA.

Integrating Digitalization and Research Data Management (RDM) intothe Curricula of Bachelor and Master Students in ChemistryFabian Fink | AK Herres-Pawlis | RWTH Aachen UniversitySMuK23 – DPG Spring Meeting | Dresden | March 23rd, 2023CC BY 4.0 ©NFDI4Chem

#### **Overview**



- 1) NFDI and NFDI4Chem Mission and Strategy
- 2) RDM Integration into a Bachelor Student's Lab Course

() ● () NFDI₄Chem

3) RDM Integration into a Master Lecture

#### **NFDI NFDI C NFDI** Chem **ENHANCE YOUR** DATA.

**NFDI and NFDI4Chem** 

# nfdi National Research Data Infrastructure

- Founded in 2018 funded by federal government and states
- Main goal: Improvement and creation of Research Data Infrastructure & Management. Provision of tools, trainings and initiation of cultural change.
- Part of federal governments digitalization strategy

#### 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)



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

#### NFDI4Chem – Who are we?





### **Composition of the Consortium**







### NFDI4Chem is embedded in an international context









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Why? What is our mission?

### **Speed of Evolution**





#### Molecules and related (Meta)Data





### **Status Quo**





#### **Our Vision**





### **Our Vision**





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### What is our Strategy?

#### Strategy





### **Involvement of the Community**





### **Involvement of the Community**





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RDM Integration into a Bachelor Student's Lab Course

#### Framework

#### Advanced inorganic lab course for undergraduate students

- Mandatory lab course for 5<sup>th</sup> semester bachelor students at RWTH Aachen
- Each winter term: 3 thematic blocks, 110 120 students
- Implementation of the Chemotion ELN (since WT20/21):
  - Synthesis of Ferrocene in the lab
  - Complete processing (planning, documentation, analysis) in the Chemotion ELN
- Learning unit on research data management (since WT20/21):
  - Short videos on the basics of RDM, FAIR principles, data management plans, metadata, and InChI & SMILES
  - Final test on RDM which students must pass in order to pass the lab course











### **Digital Documentation in the ELN**



#### Coordination chemistry < 22. B/S-IL - 00 Chemotion -Al - IUPAC, InChI, SMILES, RIN 4 + - w Chioroform-d (s): 7... w 1,23 - Layout <sup>1</sup>H --- Ay 🔃 Q P+ P- 🤍 J + J - X 1 1 J+ J+ J+ JX 10 00 Q 19(0) A 4(0) = 0(0) R 0(0 A FFI-R80 0.764 . From From **#1-44** FFI-R80 COPM . THE TREAT OF OF 0 **H1-44** Nat E FFI-R79 . Fe-Cl X 60 °C. 4.5 h **H**1-4-4 FFI-R78 × **■1-4**4 0-215.21 Carlor - 10 **≡1**-4-0 Name + E FFI-R77 $\Phi$ 2 00 - 180 °C, 4 h J. Cheminform. 2017, Start ≡1-4≪ =1.44 28/04/2021 15:00 9 (1), 54. + Type (Name Reaction Ontology) + Show 15 1 5 8 Description J. Cheminform. 2021, Name + 1H NMR 13 (1), 8. The reaction has been conducted in dry glass Sodium cyclopenta-1,3-diene (11.5 g, 130 mm Type (Chemical Met emild was added in small notions. Afterwards added to the mixture to quench the remaining Vinne 1H nuclear r fibered through diatomaceous earth and the filte Chem. Methods 2022, \*C to yield ferrocene (7.69 g, 41.3 mmol, 64% Content Normal : B I U E E X, X<sup>1</sup> > C EA H R = UV MS : 0 Purification 2 (10), e202200026. <sup>1</sup>H NMR (43 MHz, Chloroform-d [7.27 ppm], ppm) δ = 4.23 (s, 10H) **Purification Solvents** + Description Additional information for publication and BIU II X, X<sup>2</sup> Hea Datasets FerrocenNMR 1

#### **Processing of the synthesis of Ferrocene in the Chemotion ELN**

motion

<sup>20</sup> 

#### **Learning Materials and Survey among Students**

- Learning materials for using the Chemotion ELN:
  - Online documentation with introductory videos
  - In depth tutorial videos on Zenodo and YouTube
- Videos of the learning unit on RDM available on YouTube
- Survey conducted for tracking the integration of RDM in the lab course:
  - Online questionnaire using the software SoSci Survey
  - Up to 26 questions on benefits of digital documentation, the learning unit on RDM, and using the ELN in the lab course
  - WT2020/2021 survey period: 31 days, participation rate: 34% (38/111)
  - WT2021/2022 survey period: 29 days, participation rate: 34% (42/123)



ELN manual



ELN videos on YouTube



RDM videos on YouTube

### **Benefits of digital Documentation**





Do you understand the benefits of storing data digitally?





Do you think such an electronic system will make documentation faster or slower in the long run?



■ WT2020/2021 (n=37) ■ WT2021/2022 (n=40)





### **Learning Unit on Research Data Management**



Have you covered/heard any content on research data management in your studies prior to the lab course? (n=40)



Do you think that you have gained new knowledge in the learning unit "research data management"? (n=40)



- Students mainly consider the learning unit as use- and helpful overall
- Students complained about a too extensive input within the stressful winter term
  - No long-term storage of the knowledge on RDM

in my studies.

Do you think that you will need and be able to apply the contents of the learning unit "research data management" in your further studies? (n=40)



in my further studies.

### Using the ELN during the Lab Course



On a scale from 1 to 10, how difficult was the use of the ELN?



Do you think that (after a certain training period) you could use such a system for documentation?



WT2021/2022 (n=40)

WT2020/2021 (n=37)

- The number of issues (arising difficulties or problems) decreased in the latter year
  - Student's feedback as input for the further development of the software
- Students overall satisfied with the learning materials and videos for using the ELN



#### Did you have reservations about using the system or did you enjoy using it?

### **Use of the ELN in further Studies**



Would you like to learn more about the other functions of the ELN in order to be able to use it later in your bachelor or master thesis?



Would you like the ELN to be used in other lab courses in your studies and/or bachelor thesis? (n=39)



- Student's suggestions for features and a more-intuitive user interface are taken into consideration for the ELN development
- Use of an ELN is most beneficial when it is used more frequently (benefits of digital documentation become more pronounced)

#### Conclusion

- growing awareness of RDM
- higher acceptance towards ELNs
- Further needs for teaching RDM on an early stage of studies already

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### **RDM Integration into a Master Lecture**

Framework

- Optional Master lecture by Prof. Dr. Sonja Herres-Pawlis on "Sustainable Coordinative Polymerization Catalysis"
- Each winter term: 2h per week, 80 100 students, ~50 take the exam
- Topics:
  - (Second generation) bio-feedstocks
  - Bioplastics
  - Polymerization methods
  - Toxicity of catalysts
  - Industrial applications
  - Circular bio-economy
  - Research data management (as meta-competence)





- Slides for full lecture on basics of RDM (FAIR principles, DMPs, metadata, ...)
- Teaching videos on RDM:
  - General RDM videos provided by the university library
  - Specific chemistry-related RDM videos (as in Bachelor lab course)
- Case studies related to lecture's topics
  - Discussion of studies' content in general
  - Special attention to RDM in the discussion (good/bad examples)
- Self-study and further reading materials on RDM
- Basic questions on RDM in final exam





RDM videos on YouTube

### **Development of the Lecture**



#### WT18/19 and earlier

- Frontal lecture
- Interactive elements
- Bioplastic topics exclusively
- Current case studies

#### WT20/21

- Remote lecture/recordings
- Self-study materials
- Switch to specific chemistryrelated RDM videos

WT21/22

- Interactive discussions
- First integration of RDM (one lecture on RDM, general RDM videos, reading materials)

- Remote/in-person lectures
- More interactive discussions
- Current case studies with examples of good/bad RDM

#### WT19/20

29

#### **Current Development and Progress**

#### WT22/23

- RDM content known to 80% of students (from lab course)
- Self-study unit on RDM
- More current case studies (RDM)

#### Conclusion

- Students very positively accept RDM as an important meta-competence
- Chemistry-related case studies and teaching videos mediate RDM topics more effectively than general material
- Further needs for teaching RDM on an early stage of studies already



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Homepage: nfdi4chem.de REDI4Chem WIGH4Chem NFDI4Chem WIGH4Chem NFDI4Chem WIGH4Chem NFDI4Chem is an initiative to build an open and FAIR infrastructure for research data management in chemistry. @ Germany @ nfdi4chem.de I long October 2019



Great to see everyone in person at our #NFDI4chem meeting in #hannover. Thank you to everyone who participated - especially to our advisory board members. The future is bright for #FAIR #data in #chemistry. @GDCh\_aktuell @JungChemiker @NFDI\_de @NFDI4Cat Credit: TIB/C. Bierwagen



# NFDIAChem Emanne Your Dera

#### NFDI4Chem

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

#### Welcome

Dear reader,

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

With the net issue, we will star to introduce the six task areas of MFDI4Chem and the people behind them in more detail. Look forward to comprehensive reports of key topics of NFDI4Chem and NFDU. We will continue to inform you about upcoming events and report on past ones in detail. We will be excited to velcome 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 interedied in futhre topics we should cover.



#### Subscribe to our newsletter which is released every 3 months via our website!

### Acknowledgement



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## Thank you for Listening! – Any Questions?