

NFDI₄Chem Project Update Q4/2023

Recent achievements

- <u>Memorandum of Understanding with NFDI4Ing</u> about RDMO (Research Data Management Organiser) usage
- Successful Consortium Meeting 4.0 and Digital Summit in Jena (report on website)
- Chemotion ELN v1.8.1 released
- NFDI4Chem collection is now on FAIRsharing: https://fairsharing.org/5027
- Successful 2nd Editors4Chem Workshop
- Postprint Data format standards in analytical chemistry published (<u>DOI:</u> 10.5445/IR/1000150893)
- Establishment of a workshop concept for only the LabIMotion extension of Chemotion
- Faculty-wide instance of Chemotion ELN started operation at Universität Würzburg (16.10.2023)
- Successful 2nd Ontologies4Chem Workshop (Zenodo publication)



Project Update Q4/2023

TA1

- MoU with 4Ing about RDMO
- Successful CM4.0 in Jena (<u>report</u>)
- 84 % of funds were approved for carryover to 2024
- <u>Activity Update on the</u> <u>documentation of cross-cutting</u> <u>activities</u> published
- Preparation of Community Workshop in February 2024

TA₂

- Chemotion ELN <u>v1.8.1</u> released
- <u>Chemotion test instance</u> features tagged for <u>v1.8.1</u> & <u>v1.9</u>:
 - Sample inventory label
 - o Cell line element
- ChemSpectra now allows to add reference values for analysed data and reports peaks for XRD spectra.

TA3

- NFDI4Chem collection is now on <u>FAIRsharing</u>
- Conference attendance with poster (IDW 2023), presentation, workshop (Conf. on Safety of Adv. Mat.)
- Consideration of adding Sciflection to the <u>list of</u> recommended repos

TA4

- <u>2nd Editors4Chem Workshop</u> took place on 2nd November
- Postprint Data format standards in analytical chemistry published in KITOpen (DOI)
- Converter service: Development of REST API of the converter service in OpenAPI specification is in process

TA₅

- Workshop concept for LabIMotion
- Faculty-wide Chemotion instance at Uni Würzburg started
- KB team established
- national and international Chemotion outreach activities and workshops
- FAIR4Chem award: 10 subm.
- New Flyer (Hitchhiker's Guide)

TA₆

- Successful 2nd Ontologies4Chem Workshop (<u>Zenodo publication</u>)
- VIBSO: switch to TBox
- implementation of new molecular view page in Search Service
- BioSchemaOrg extending CKAN Schema for NFDI4Chem
- participation in various IAM4NFDI activities





Project Update Q4/2023

Upcoming events/meetings

- 18.01.2024: Meeting with Bruker Optics on data (format) standards for optical spectroscopy
- 31.01. 01.02.2024: Community Event of DALIA/NFDI-Edutrain
- 14. 16.02.2024: Young Chemists Summit Salzburg (public)
- 26.02.2024 NFDI4Chem Community Workshop in Mainz (public)
- 11. 13.03.2024: ADUC in Aachen (public)
- 13. 16.03.2024: Frühjahrssymposium of the GDCh Young Chemical society (public)
- 17. 21.03.2024: Bunsen Tagung (public)
- 10.04.2024 NFDI4Chem Consortium Meeting 4.5 online (internal)
- <u>Chemotion ELN Q&A session</u>: every second Thursday (3pm)
- <u>Chemotion Stammtisch</u>: last Friday of every month (2:00 PM)
- Various TA meetings, see specific invitations and individual flash reports

Announcements

- A4 Data Pledge continues: pledge your datasets from previous, current or upcoming publications through our <u>survey form</u>
- Join the NFDI Verein: https://www.nfdi.de/verein