

NFDI₄Chem Project Update Q1/2024

Recent achievements

- <u>RPTU</u> joined NFDI4Chem Welcome!
- Successful <u>Community Workshop</u> on 26th February
- Chemotion ELN v1.9.0 released
- Chemspectra backend <u>v.1.1.1</u> and frontend <u>v.1.2.1</u> released
- RADAR4Chem, RADAR4Culture, and NFDI4Chem collection now on FAIRsharing
- Deliverable 3.2.3 "CTS certification for selected repositories" closed
- Information about repos updated on forschungsdaten.info
- New InChI version online v1.07 (https://github.com/IUPAC-InChI/InChI Dev)
- MS converter in repo ready with REST API (https://git.rwth-aachen.de/linsherpa/ms_converter)
- FAIR4Chem Award awarded to Robin Lenz @ FJS
- Chemiedozententagung Aachen 11.-13.03.: Booth & 2 NFDI4Chem Workshops
- 1st LabIMotion workshop (07.03.) positively received
- Graph visualizationin Terminology Service → also support SKOS
- Search Service: Bulk Harvesting possible via JSON file dump/upload; implemented on MassBank
- Contribution to <u>IUPAC FAIR Chemistry Cookbook</u> with 2 articles about <u>Repositories & Search Service</u> and Terminonlogy Service



Project Update Q1/2024

TA1

- Annual report of expenses
- Preparation for renewal proposal, incl. DFG Datasheet
- TA1 joined NFDI Task Force Governance & Sustainability
- 'Declaration of joint processing of data' signed by co-applicants
- RocketChat runs now on (free) community license

TA₂

- Chemotion 1.9.0 new features: extended search feature, default ketcher2 configs, and more
- Chemspectra new features: add new data types without update, report peaks from XRD function, and more
- Automated (docker) image builder for Chemotion ELN

TA3

- part of <u>FAIRsharing Community</u> <u>Champions Programme</u>
- Paper on "Beyond FAIR" sent to CODATA Science Journal
- Article for IUPAC chem cookbook on repo federation sent
- various RADAR software releases

TA4

- new members from RPTU: MiChI for photochemistry
- partner from IPHT will lead MiChI for RAMAN spectroscopy
- Revision of KB page within section on data publishing

TA5

- attendance/ presentations in 8 conferences (inter)national
- 2 RDM workshops
- 3 Chemotion workshops
- increased cooperation with PSDI (UK)
- Own NFDI4Chem Column in Nachrichten aus der Chemie

TA₆

- "Guidance how to use IUPAC Goldbook (...)" finalized
- VIBSO: defining Raman Spectroscopy types
- nmrCV migrates to ODK-based setup
- position paper to draft of Research Data Act



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Upcoming events/meetings

- Consortium Meeting 4.5: 10.04.2024, online
- MADICES Cecam Workshop: 22. 25.04.2024, Berlin
- Meeting of the Bio-Chem-Geo-NFDI-Helpdesks: 27. 28.05.2024, Bremen
- EuChemS (incl. joint symposium with PSDI): 07. 11.07.2024, Dublin
- Consortium Meeting 5.0: 10. 11.09.2024, Halle (Saale)
- <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