

Project Update Q3/2022

Recent achievements

- Request for "Mittelübertrag" to 23 completed and submitted to DFG
- Uni Stuttgart (Pleiss) joins the consortium and Uni Köln has left the consortium (31.12.2021)
- Data-converter ELN integration; Chemspectra documentation (docusaurus)
- Device Integration: Full integration of SEC-THF, SEC-DMAC, LowTemp. DSC, FT-IR.
- Decision tree for the KB-article "how to choose the right repository" uploaded to Media4 Timespin
- MIChI: Bioschemas implementation in nmrXiv
- Author Guidelines manuscript: Publication Standards finalized. Submission Journal: Pure Appl. Chem.; Dataset: RADAR4Chem
- Several presentations of Knowledge Base and NFDI4Chem as well as Workshops (FAIR RDM and Chemotion)
- Job advertisement for PR manager published
- Sonja Herres-Pawlis elected as deputy spokesperson for section training & education
- WG Error culture in science established (section training & education)
- Paper on <u>Guidelines for Sharing in the ELN Chemotion</u> published in Chemistry Methods
- 1st Ontologies4Chem Workshop (Event <u>DOI: 10.25798/frnp-sn04</u>) and completion of NFDI4Chem TS 2.0
- Successful harvesting from Chemotion (direct OAI) & Radar(DC)



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TA1

- Request for "Mittelübertrag" to 2023 completed and submitted to DFG
- Preparation CM 3.0; registration closed
- Uni Stuttgart / Pleiss joins the consortium

TA2

- Chemotion_ELN v1.4.0 refactoring ongoing
- Server side molecule rendering service
- CLI tool for development env

TA3

 Decision tree for the KB-article "how to choose the right repository" uploaded to Media4 Timespin

TA4

- TGF is back and will take over TA4 PM from DR
- LbE: Assessment template created; 2 ext. contributors acquired; Publication of three datasets by Dieter Sicker and Stefan Berger in RADAR4Chem

TA₅

- Job advertisement for PR manager published
- Sonja Herres-Pawlis elected as deputy spokesperson in section training & education
- Ongoing progress of TUCAN and next InChI version

TA6

- Added TSV edit pipeline for Vibration Spectroscopy Ontology
- Meeting with IUPAC wrt using GoldBook as definition source for chemical ontologies



NFDI₄Chem Project Update Q3/2022

Upcoming events/meetings

- <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
- FAIR Convergence Symposium 2022 (24 26 Oct. 2022) Leiden, NL
- FD02022 Conference 26 28 Oct. 2022 Leiden, NL
- 1st <u>BioHackathon</u> (Lutherstadt Wittenberg Leucorea) 12-16 December 2022

Announcements

- TA4 Data Pledge continues: pledge your datasets from previous, current or upcoming publications through our survey form
- Join the NFDI Verein: https://www.nfdi.de/verein