

Project Update Q2/2023

Recent achievements

- T1.1.1: Admission of BAM as participating institution acc. BLV approved by DFG
- Report for D1.3.1 finished (The NFDI4Chem portal)
- Chemotion: Implementation started on new cell line element to introduce biochemistry features
- Chemotion ELN v1.6.1 is released
- Chemotion test instance is now ready for testing for external users. Instance include features tagged for v1.7
- ChemCLI <u>v0.2</u> released; started with providing cloud-based auxiliary service endpoints to internal developers
- 4 Abstracts for CORDI-Conference have been accepted for presentation; additionally 2 posters accepted
- First implementations of ELN-Repo data exchange (to RADAR4Chem, RADAR4KIT)
- Deliverable 4.5.1 (Report on FAIRness of datasets) is ready to be published.
- TA4: M4.5 started a Pilot with Beilstein Institute on metadata enrichment of articles
- Chemistry Data Days more than 90 participants from various backgrounds outside of the "RDM-bubble" have joined
- Exchange Workshop 4Cat: talk from Pedro Mendez, followed by cross-consortia breakout rooms on topics such as training, metadata & ontologies and ELNs & repositories
- Launch of public <u>TS demo server</u> for testing notes feature
 - Demo Features:
 - Note system for ontology/term/property/individual
 - Term request/issue report for Ontologies hosted on Github
 - List of Git issues for an ontology



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TA1

- Assignment of BAM and Uni Stuttgart to Consortium acc. statute requested
- SOP for Offboarding completed
- T1.1.2: regular quarterly activities for budget request & transfers
- T1.2.1 & T1.2.2: ongoing preparation Consortium Meeting 4.0
- Update of budget plan

TA₂

- Implementation begun on new vessel element for FAIR reaction process workflow
- Implementation of experiment / catalysis feature in progress: work on front- and backend; updates and bug fixes in related dependencies

TA3

- Application for FAIRness assessment challenge for RADAR to FAIR-IMPACT has been submitted.
- Interview results of VibSpecDB collected
- Ongoing development of a modernized MassBank infrastructure

TA4

- 13th TA4 TelCo on 2023-06-12
- Manuscript submitted to CoRDI and Semantics
- M4.3 on Raw Data Converter Services collected a large body of MS test data, which will be used to improve existing infrastructure for conversion.
- Draft of NMR MIChI available to be discussed at NMR Task Force Meeting in Jena

TA5

- Conferences attendance; Chemotion Demos; NFDI4Chem Introductory Talks; RDM und InChi Workshops
- Presentation on Error Cultures in the JCF forum for mental health
- Second community survey closed on 15.04.2023
- Steady increase of social media followers across all platforms

TA6

- TS Paper submitted for SEMANTICS Conference
- VIBSO 2 dev calls
- Section Metadata: WG Ontology Hamonization & Mapping
- participation in <u>SSSOM</u> & <u>FAIR-Impact</u> workshop, <u>OntoSummit'23</u>
- Progress analysis of the BioSchema JSON schema on nmrXiv & Massbank (submitted a paper for the SEMANTiCS)





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Upcoming events/meetings

- Chemotion Workshops: 27.07. online, 11.07. TUM, 26.-27.09. Würzburg
- 4Chem Workshop at Klausurtagung JCF (Wuppertal, 25.-27.08.)
- ACS Fall (San Francisco, 13.-17.08., Co-chairing 2 sessions and multiple talks)
- IUPAC Chains (The Hague, 20.-25.08.)
- WiFo (Leipzig, 04.-06.09.)
- CoRDI (Karlsruhe, 12.-14.09.)
- Python Programming Course for Chemists (Aachen, 18.-20.09.)
- 20.-22.09. SEMANTICS Conference (public)
- IDW 2023, Salzburg 23-26 October
- Consortium Meeting 4.0 (Jena) on 22.-23.11.2023

Announcements

- Admission of <u>BAM</u> to NFDI4Chem according to BLV approved by DFG
- NFDI e.V. Code of Conduct now adopted
- Inclusion of German language versions on Knowledge Base and Website