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Embedding RADAR4Chem into NFDI

Integrating Base4NFDI services into a trusted research data repository for chemistry

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Abstract

RADAR4Chem is a discipline-specific research data repository developed to meet the needs of the chemical sciences within the framework of the National Research Data Infrastructure (NFDI). It is based on the generic repository **RADAR**, developed and operated by FIZ Karlsruhe - Leibniz Institute for Infrastructure [1]. Our engagement in many NFDI consortia has already resulted in different RADAR variants¹ that are tailored to the specific requirements of the various scientific communities. As a core repository of the NFDI4Chem consortium, RADAR4Chem enables the publication, long-term preservation, and sharing of FAIR (Findable, Accessible, Interoperable, Reusable) data. Its functional evolution, especially its ongoing integration with basic NFDI services (Base4NFDI), strengthens RADAR4Chem's role in supporting trustworthy and standards-compliant digital research workflows and fosters its chemistry-specific focus.

A key integration is the implementation of **Terminology Services 4 NFDI (TS4NFDI)**, which RADAR4Chem has achieved as an incubator project. TS4NFDI provides access to well-maintained ontologies and controlled vocabularies relevant - but not limited - to chemistry, ensuring semantic consistency and enabling machine-readable data annotation [2]. Through TS4NFDI, RADAR4Chem facilitates metadata annotation and improves the interoperability and findability of datasets across disciplinary and institutional boundaries.

To better address domain-specific needs of chemistry, RADAR4Chem is being continuously enhanced to support **chemistry-relevant metadata standards**, particularly Minimum Information about Chemical Investigation (**MICHI**). These community-driven profiles, being developed through a collaborative effort within the NFDI4Chem consortium, supported by IUPAC, defines essential metadata fields across common chemical domains [3]. By embedding MICHI profiles into RADAR4Chem, the repository enables more accurate and structured metadata collection, thus supporting reproducibility, reuse, and compliance with publisher and funder requirements.

In alignment with NFDI-wide efforts to streamline authentication and access, RADAR4Chem supports federated Identity and Access Management (IAM) via the **IAM4NFDI service and**

¹ e. g. RADAR4Culture for NFDI4Culture, RADAR4Memory for NFDI4Memory

its RegApp system. This allows researchers to safely log in through their institutional credentials, thus avoiding local account management and promoting seamless integration across services [4]. In future, the AAI (Authentication and Authorisation Infrastructure) model will also support RADAR4Chem's role-based access control and facilitate collaborative curation management.

Furthermore, RADAR4Chem is linked with the Research Data Management Organiser (RDMO) to support the creation and exchange of structured data management plans [5]. This integration is aligned with the goals of the **DMP4NFDI initiative**, which aims to structure and lifecycle standardisation of data management planning across domains [6], with NFDI4Chem participating as an incubator project. By means of this connection, metadata defined in **RDMO NFDI4Chem**, as a chemistry-specific instance, can be seamlessly transferred to RADAR4Chem, enabling more efficient workflows with minimal redundancy.

A similar transfer is possible by RADAR4Chem's connection to the **Chemotion Electronic Lab Notebook (ELN)**, allowing chemists to handle their data throughout the data lifecycle, from planning and annotation to publication and long-term preservation.

Our poster illustrates how technical and semantic integrations establish RADAR4Chem as a robust and interoperable repository service aligned with the goals of both NFDI4Chem [7] and NFDI. It streamlines data management workflows, enhances interoperability, and supports effective dissemination and preservation of research data, ensuring that outputs remain documented, accessible, reusable, and fulfill the FAIR principles.

Keywords: RADAR4Chem, Research Data Repository, NFDI4Chem, FAIR data, Base4NFDI, Terminology, TS4NFDI, MICHI, IAM4NFDI, DMP4NFDI

Resources:

- RADAR4Chem. <http://doi.org/10.17616/R31NJNAY> Research data publishing service for the chemistry community.
- RADAR. <http://doi.org/10.17616/R3ZX96> Repository for archiving and publishing research data from completed scientific studies and projects.
- NFDI4Chem Core Repositories. https://knowledgebase.nfdi4chem.de/knowledge_base/docs/choose_repository The NFDI4Chem Knowledge Base provides information and recommendations to digitalise all key steps of chemical research and e. g. lists NFDI4Chem Core Repositories.
- Basic Services for NFDI (Base4NFDI). <https://base4nfdi.de/> Foundational, cross-disciplinary services and infrastructure to support data management across all consortia within the NFDI.
- Terminology Services for the German National Research Data Infrastructure (TS4NFDI). <https://base4nfdi.de/projects/ts4nfdi> Cross domain service for the provision, curation, development, harmonization and mapping of terminologies.
- Identity & Access Management for the German National Research Data Infrastructure (IAM4NFDI). <https://base4nfdi.de/projects/iam4nfdi> Secure, federated system to manage user identities and access rights across all NFDI consortia.
- Research Data Management Organiser (RDMO). <https://rdmorganiser.github.io/> Software that supports research projects in the planning, implementation and administration of all research data management tasks.

- Data Management Plans for the German National Research Data Infrastructure (DMP4NFDI) <https://base4nfdi.de/projects/dmp4nfdi> Services and guidance to create, manage, and standardize data management plans across NFDI consortia.
- RDMO NFDI4Chem. <https://rdmo.nfdi4chem.de/> Customized version of RDMO tailored to support researchers in chemistry with creating and managing data management plans.
- Chemotion Electronic Lab Notebook (ELN). <https://chemotion.net/docs/eln> Digital platform to support chemists in documenting, managing, and sharing their laboratory research data.

Author Contributions

- Felix Bach: Conceptualisation, Investigation, Writing – original draft, review & editing
- Kerstin Soltau: Conceptualisation, Resources, Validation, Writing – review & editing
- Stefan Hofmann: Software, Methodology, Writing – review & editing
- Christian Bonatto Minella: Investigation, Validation, Writing – review & editing
- Sergio Pollo Vázquez: Software, Methodology, Writing – review & editing

The authors have applied the CRediT (Contributor Roles Taxonomy) to define individual contributions.

Competing Interests

The authors declare that they have no competing interests.

Funding

This work was funded by the German Research Foundation (DFG) within the framework of the National Research Data Infrastructure (NFDI) programme – project number 441958208, NFDI4Chem.

Acknowledgement

The authors thank NFDI4Chem and FIZ Karlsruhe for their support, as well as the Base4NFDI initiative for their basic services (TS4NFDI, IAM4NFDI, DMP4NFDI) which enhance the integration potential of RADAR4Chem. Special thanks to the RDMO developers for collaboration in establishing RDMO integration and export templates.

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