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Activity Update
Report on 2nd Ontologies4Chem Workshop 2023

TA6 – Synergies

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Gefördert durch Deutsche Forschungsgemeinschaft (DFG)
Projektnummer: 441958208
Programm: Nationale Forschungsdateninfrastruktur

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Executive Summary

The 2nd Onotologies4Chem Workshop brought together experts from various domains to address the development, curation, and application of ontologies in chemistry and related fields. The discussions and presentations highlighted the complexities and challenges in the sustainable curation of chemical ontologies. A significant emphasis was placed on the necessity of involving more domain experts in the development and curation process to address these challenges effectively. Significant advancements in tools and services were showcased, including the NFDI4Chem Terminology Service, which aims to simplify ontology development and attract more domain experts. A key focus of the workshop was on the ongoing efforts to create FAIR metadata for ontologies. These efforts are crucial in improving the standardization, interoperability, and overall quality of ontologies and their curation processes. The integration of ontologies into data annotation tools, such as SWATE and Ontomaton, was discussed as a user-friendly approach for generating semantically rich research data, thereby demonstrating the practical applications and benefits of ontologies in research. Looking toward the future, the workshop identified the need for further collaboration between domain and ontology experts and the broader integration of ontologies into various research tools. This is seen as a vital step in advancing the field and addressing the overarching view of semantically linked research data in both academia and industry. The workshop concluded with a consensus on the importance of increased collaborative efforts, enhanced joint communication strategies, and the sharing of success stories to engage more domain experts in the field of ontologies in chemistry.
The recordings of the workshop can be accessed on the NFDI4Chem YouTube channel.

Project objectives

With this deliverable, the project has reached/this deliverable has contributed to the following objectives:

a) O6.1 Users can search for research data across distributed data sources of federated NFDI4Chem repositories and linked repositories of the NFDI.
b) O6.2 Scientists can use and access NFDI4Chem's services and components in a uniform and user-friendly manner.

Detailed report on the activity

Report for Day 1

Day one of the workshop was focused on discussing existing chemical ontologies in terms of how they can be explored, how far they have been updated since the last workshop, which are suitable for reuse in the NFDI4Cat context, and how their gaps can be addressed by involving domain experts with little to no ontology background in the development process but with canonical knowledge resources like the IUPAC Gold Book.

NFDI4Chem Terminology Service Updates

The workshop commenced with a comprehensive presentation on the latest advancements in the NFDI4Chem Terminology Service (TS) towards a tool suite for ontology curation and development, particularly spotlighting the integration of notes and GitHub features. These enhancements facilitate more effective ontology curation.[1] The GitHub integration allows users to conveniently list and address open issues directly within the TS, fostering a more streamlined process for submitting new term requests or questions. A live demonstration showcased the utility of the notes feature to share insights about an ontology within the TS as an additional layer of ontology metadata, thereby promoting knowledge sharing. This session built upon the challenges identified in last year's discussions regarding the maintenance of chemical ontologies, particularly their intricate connections within larger ontological frameworks. Necessary and relevant information needed for ontology maintenance is scattered in multiple places. The presented solutions, including the ability to browse the ontologies and discuss their characteristics, dependencies, and relations through attached notes and integrated issue tracking, directly address the need for a comprehensive view through a centralized and accessible platform for holistic ontology maintenance. Further discussions elucidated the indexing workflow and distinct features of the NFDI4Chem Terminology Service compared to the OLS by EBI, from which the source code of the TS backend is derived from. Development teams from both TS and EBI OLS are in contact, evaluating potential future synergies in a collaborative development process. It was pointed out that the individual roadmaps, user communities, and resulting priorities have to be considered. The notes feature and additional metadata on ontologies are exclusive to the NFDI4Chem TS. Nevertheless, the potential for merging these developments back into the OLS source code was pointed out.

The discussion clarified the relationship between the content of the NFDI4Chem TS and OLS. It was emphasized that the NFDI4Chem TS operates independently. Indexed ontologies are not forked by TS. Instead, any notes or comments made on these ontologies within the TS are treated as additional, standalone metadata. This approach maintains the integrity and autonomy of the original ontology sources. Furthermore, it was pointed out that these notes could potentially be integrated back into the original ontology source code as annotations, should the ontology curators find them valuable. This feature exemplifies the system's flexibility and the potential for cross-platform metadata utilization, as other systems can access and leverage this enriched metadata through the TS API.

NFDI4Cat Ontology Analysis

Building upon the initial analysis introduced at last year's Ontologies4Chem workshop, NFDI4Cat has made significant strides in examining the ontology landscape in catalysis, a domain sharing considerable overlap with NFDI4Chem. This year, Alexander Behr showcased the final findings of this research.[2] The preliminary work had already underscored the challenge of identifying suitable ontologies for the catalysis domain, given its interdisciplinary nature and the dispersion of relevant concepts across various ontologies. To date, there are no existing ontologies that perfectly align with the specific use

cases of NFDI4Cat. Leveraging the groundwork laid by NFDI4Chem's ontology landscape analysis [3] and NFDI4Ing's ontology development [4], the team embarked on a comprehensive search through BioPortal and OLS. This effort resulted in the identification of 30 ontologies, 23 of which were selected for a detailed evaluation. The in-depth analysis involved assessing the conceptual overlap of these 23 ontologies through term IRI and lexical label/synonym matching, examining the quality of available ontology metadata, and evaluating their logical consistency. The crux of this analysis, however, was to determine the extent to which these ontologies encompass 14 specific subdomains in catalysis, such as Homogenous Catalysis, Process Modeling, and Heat, Transport, and Kinetic Data. This was achieved by manually classifying the presence and relevance of concepts related to these subdomains within each ontology. A radar plot visually representing this subdomain coverage was presented, highlighting the existing conceptual gaps. Both the methodology and the results of this comprehensive analysis are openly accessible on GitHub.[5] In response to the conceptual gaps identified, the NFDI4Cat domain experts have initiated the development of a SKOS vocabulary, named Voc4Cat, employing an automated workflow designed by domain specialists.[6] The NFDI4Cat ontology team's future agenda includes further refinement of their ontology collection and exploring the feasibility of automatic mapping between concepts in Voc4Cat and those in existing ontologies. This approach is anticipated to enhance the efficiency of ontology development for the required concepts."

Ontologies4Chem - Status Updates

Day one of the workshop concluded with a series of presentations delving into the latest developments, challenges, and future directions in enhancing the chemical ontology landscape. Carlos Moreno delivered an insightful update on the progress of the Chemical Entities of Biological Interest (ChEBI) ontology. The forthcoming ChEBI 2.0 version is set to resolve numerous existing issues by adopting a modernized software stack, including PostgreSQL and ROBOT, and aligning with OBO best practices for the release of different serializations. This version also boasts improved build automation, quality control, and the introduction of monthly BETA releases for early adopters. Additionally, all object properties have been replaced by newly created RO properties to standardize with OBO. The team is currently working on how to best model annotation properties, such as charge and mass, in a way that is both consistent and extensible.

Following this, Javier Acosta presented the scope and use case of the eNanoMapper Ontology (ENMO) [7], which has been recently added to the NFDI4chem collection. ENMO, crucial to the eNanoMapper project, employs modularization through tools like ROBOT. The team is now working on enhancing the build pipeline using the Ontology Development Kit (ODK) [9] to ensure logically sound imports from other ontologies, with plans for SSSOM Mappings and redefining certain entities and concepts. Acosta also presented a brief status update on the development progress of the Chemical Information Ontology (CHEMINF) [10] which unfortunately has encountered stagnation due to limited resources, which has prevented addressing issues identified last year. A suggestion was made by NFDI4Chem to transition CHEMINF to an ODK-based repository and workflow for easier external contributions and fixes of many open issues will be discussed in the CHEMINF development team, to see if some priorities can be shifted to accomplish this goal.

Philip Strömert provided updates on the Royal Chemistry Society's ontologies - CHMO, RXNO, and MOP, and briefly introduced the PROcess Chemistry Ontology (PROCO).[11] Despite PROCO's applicability in describing process chemistry concerning concepts like product quality, process robustness, economics, environmental sustainability, regulatory compliance, and safety, its integration with other OBO Foundry-based chemical ontologies remains unclear due to dependencies on the Allotrope Foundation Ontology Suite and limited documentation. Therefore, a more in-depth community analysis or enhanced collaboration with the Allotrope Foundation was proposed. Strömert also summarized ongoing efforts to harmonize CHMO with OBI and the previous NFDI4Chem work addressing the migration of RXNO and MOP to an ODK-based workflow.

A significant takeaway from these presentations was the persistent challenge of the scarcity of skilled personnel in the field of chemical ontology development and curation. Johannes Hunold's flash talk addressed this issue by demonstrating how the lessons learned from NFDI4Chem's ongoing ontology work have led to improvements in the NFDI4Chem TS that were presented at the beginning of the workshop.[12] In a similar vein, David Linke from NFDI4Cat discussed their automated GitHub workflow for developing the Voc4Cat SKOS vocabulary, which only requires domain experts to manually curate Excel files and is adaptable for use in other contexts.[13]

Noura Rayya and Philip Strömert's presentation centered on the use case example of integrating chemical ontologies into metadata descriptions of NMR spectroscopy datasets in the nmrXiv data repository. They discussed the conceptual overlaps, issues, and gaps between the Nuclear Magnetic Resonance CV (nmrCV) and the Chemical Methods Ontology (CHMO) and how these could be addressed.[14] The primary goal was to gather community feedback on the best approach forward, whether that involves rebooting nmrCV, minting new equivalent classes in CHMO, or developing a new SKOS vocabulary utilizing the NFDI4Cat workflow. While CHMO maintainer Colin Batchelor is open to long-term improvements, there was a partial consensus on a short-term nmrCV reboot with reduced axiomatization as an easier option. The idea of using an SKOS vocabulary as an interim solution to quickly mint needed new concepts did not receive much popularity.

The final talk of the day continued the discussion from the previous year's workshop about using The IUPAC Compendium of Chemical Terminology (the "Gold Book") as a canonical source for writing natural language term definitions in chemical ontologies.[15] While some ontologies already reference the Gold Book in some form in their term metadata, a common best practice on how to reuse and cite the IUPAC definitions in formal ontologies is yet to be established. Representatives from IUPAC and NFDI4Chem have made progress in this area, presenting a draft containing guidelines to collect valuable community feedback. Licensing concerns raised during the discussion were effectively addressed, and a plan was set to circulate the draft guidelines post-workshop for a more thorough review through an open call for comments.

Report for Day 2

The second day of the workshop commenced with a succinct recapitulation of the key insights and discussions from the first day, setting the stage for the day's agenda. The primary focus shifted to exploring the realms of ontology metadata and the various applications leveraging ontologies for annotating research data. These sessions delved into the intricacies of how ontology metadata can be effectively managed, curated, and utilized, highlighting the latest advancements and challenges in this domain. Furthermore, practical demonstrations and discussions on applications showcased the real-world implications and benefits of using ontologies to enhance the accuracy and depth of research data annotation. The workshop culminated in a final discussion round, where participants collectively reflected on the outcomes and learnings of the workshop. This session provided a platform for an open and constructive exchange of ideas about future directions and next steps in the field of ontologies in chemistry and related disciplines. The participants shared their ideas and discussed potential strategies to overcome existing challenges.

Ontology Metadata Requirements

The second day of the workshop opened with a focus on the critical topic of Ontology Metadata Requirements. The initial talk, delivered by Susanne Arndt and Philip Strömert, delved into the essential aspects necessary for effectively indexing ontologies in registries and look-up services.[16] This included discussions on evaluating and validating the quality, FAIRness, and use-case applicability of ontologies for annotating FAIR research data. They introduced a draft of an ontology-level metadata schema and a validation approach, intended for use in an automated indexing pipeline of the TIB TS. Their presentation emphasized the significance of adhering to existing recommendations [17], best practices [18], and formalizations [19] in ontology metadata, and the methodologies for validating such metadata using tools like SPARQL or SHACL. They highlighted the need for a universally accepted ontology metadata standard that accommodates different use case profiles, including term-level metadata. In the context of assessing the quality and domain-specific applicability of ontologies, Hendrik Borgelt briefly discussed the ontology metadata requirements from the NFDI4Cat perspective.

Charles Hoyt's talk furthered the discourse on standardized ontology metadata. He underscored the necessity for standardized prefixes, URIs, and compact URIs (CURIES) for consistent referencing of ontologies or terms and for facilitating semantic mappings.[20] He explained the role of the Bioregistry, a registry for ontologies and databases as well as a meta-registry that indexes other ontology registries. Bioregistry can be used for normalizing ontology prefixes across various applications. Hoyt discussed how standardized CURIES of ontology terms can aid in creating and curating semantic mappings between chemical ontologies and databases. Given the depth and breadth of information covered, including links and calls to action for NFDI4Chem and other NFDI consortia, Hoyt’s presentation was seen as potentially impactful for the development of ontology-based tooling and related efforts within these consortia.

The ensuing discussions of these two presentations revolved mostly around the question of what to do when needed metadata is not present in the ontology source code and how to curate it in external platforms. Having had representatives of some of such services within the audience allowed for a fruitful exchange of experiences and links to ongoing work in this direction. There was a consensus on the need for collaborative efforts in establishing a flexible yet unified ontology metadata standard. However, it was also pointed out that there is a need to provide better tooling and incentives that will allow such externally curated metadata to be fed back into ontology source codes.

Ontology-Driven (Meta)data Annotation

The workshop then transitioned to a series of talks highlighting practical tools and pragmatic workflows for research data annotation driven by ontologies. Angela Kranz initiated this segment by introducing SWATE, an annotation tool developed by the NFDI consortium DATAplant as part of their Annotated Research Context (ARC) framework. SWATE, designed as a Microsoft Excel plugin, enables researchers to annotate tabular data, particularly column headers, with ontology terms through an intuitive interface. Steffen Neumann followed with a presentation on Ontomaton, a tool similar to SWATE but tailored for Google spreadsheets.[21] Unlike SWATE, which relies on the ontologies indexed in DATAplant's ARC framework database, Ontomaton leverages the APIs of EBI's Ontology Look-Up Service [22], NCBO's BioPortal [23] and the Linked Open Vocabularies (LOV) registry [24] for term look-up, with the capability to restrict term searches to specific ontologies in certain cells.

Venkata Chandrasekhar Nainala shifted the focus to software developers by showcasing the Ontology Elements, an HTML web component library designed to normalize and semantify text input in applications like electronic lab notebooks or data repositories.[25] This software library interfaces with the NFDI4Chem TS API by default and can be configured to use EBI's OLS API, facilitating the search and selection of ontology terms or to map entities of a passage text to their ontological representation directly within the text input field. The session continued with two flash talks addressing the aggregation of chemistry-specific datasets from various repositories in a FAIR manner utilizing metadata that is based on a schema that requires the use of ontology terms to describe the used measurement technique and other attributes. Steffen Neumann discussed the application of specific Bioschema.org profiles for metadata schemata in chemistry [26], while Bhavin Katabathuni demonstrated its implementation in the NFDI4Chem Search Service, using the Massbank repository as an example.[27]

Subsequent discussions raised concerns about the reliance on proprietary software like Excel and Google Sheets in the context of SWATE and Ontomaton for FAIR research data management (RDM) workflows. In response, DATAplant is considering transforming SWATE into a standalone application. It was pointed out that the XLSX format can be read and edited with non-proprietary tools and that long-term experiences with Microsoft's COM automation interface suggest a rather stable compatibility. Other aspects that were discussed revolved around the set of ontologies from which terms can be chosen and the limited term metadata that is provided within the presented tools. Given that broader terms

may exist in multiple indexed ontologies, there was a consensus on the need for users to have prior knowledge about which terms to select from which ontology. To address this, participants suggested providing links to additional term metadata from the lookup services within these tools. It was also noted that since such tools rely on multiple API calls, the speed of these APIs must be fast enough to allow for smooth user experiences. The audience also provided helpful feedback in terms of links to other projects with which the Bioschema.org-based approach used by the NFDI4Chem Search Service could be improved in the future.

Final discussion

The workshop's concluding discussion session focused primarily on addressing the critical issue of limited domain experts contributing to the development and curation of chemical ontologies. This challenge was repeatedly emphasized throughout the workshop, particularly in relation to the NFDI4Chem Terminology Service (TS), which seeks to mitigate this gap by offering an intuitive interface for easier accessibility and usability of curation and development features. Despite these efforts, audience feedback highlighted a significant need for more effective communication regarding the vital role of ontologies in achieving FAIR research data. One of the key themes that emerged from the discussions was the apparent lack of incentives for domain experts to engage more deeply with ontologies, either their application or their development and curation. Such involvements are still not considered relevant enough compared to all the other tasks associated with researchers' daily work. There is a pressing need to showcase the tangible benefits of ontology usage, demonstrating how they can streamline processes in daily workflows, such as through ontology-driven applications for electronic lab notebooks, data repositories, or database search services. The present workshop was acknowledged as an important step in this direction by bringing together different stakeholders and providing valuable insights and venues for discussion.

Looking ahead, the participants recognized the importance of continuing this series of workshops to maintain momentum and foster ongoing collaboration. Future initiatives such as hackathons were proposed to actively enhance the quality of existing chemical ontologies by addressing some of the issues identified during the presentations. These could provide hands-on opportunities for domain experts to contribute directly to ontology improvements. The efforts surrounding the IUPAC Gold Book guidelines for ontology development and curation were met with positive feedback. The consensus was to extend a call for comments to a wider range of stakeholders for the first version of the guidelines, ensuring these are refined to meet the needs of the broader chemical community effectively.

Conclusion and Outlook

The 2nd Ontology Workshop highlighted the critical need for enhanced collaboration, the development of more efficient tools and workflows, and the implementation of strategic communication to advance the understanding and application of ontologies in chemical research. Bridging the gap between domain expertise and ontology development is

essential for the community to fully leverage ontologies, thus improving and streamlining research data management and utilization. The challenges faced in curating key chemical ontologies, such as CHEMINF, CHMO, MOP, and RXNO, were clearly illustrated during the workshop. Recent advancements in services and tools, notably the NFDI4Chem Terminology Service, are geared towards reducing entry barriers, thereby encouraging domain experts to engage in ontology development and curation. The workshop emphasized the importance of adopting workflow tools like the Ontology Development Kit (ODK) across different ontology projects to facilitate community contributions. Efforts towards creating FAIR (Findable, Accessible, Interoperable, and Reusable) metadata for ontologies are expected to significantly improve standardization, interoperability, and the overall quality of ontologies and their curation processes in the long term. The prospect of the IUPAC Gold Book as a canonical source for term definitions in chemical ontologies also supports standardization by authoritative definitions, thereby enhancing the clarity and consistency across chemical ontologies. Although only briefly mentioned, the potential for collaboration between the open ontologies community and initiatives like the Allotrope Foundation should be explored further. This could provide a more comprehensive perspective on the semantic linking of research data across both academic and industrial landscapes. The integration of ontologies into annotation tools such as SWATE and Ontomaton, and their incorporation into the annotation workflows of data repositories and electronic lab notebooks (ELNs), is crucial for enhancing the application of ontologies. This will help generate semantically rich research data and demonstrate their value to the broader research community. To truly engage domain experts and foster their participation, it is essential to collate and showcase success stories that highlight the positive impact of semantically rich research data in the field of chemistry. These narratives will serve as powerful examples of the benefits of ontology application, inspiring more experts to contribute to this evolving field.

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Appendix

- YouTube link to the workshop recordings: https://www.youtube.com/playlist?list=PLlTKDYkC1Ls_Vvym6FY1hdDzA1VcPGu9i