Fórum de Gestão de Dados de Investigação

Estudo bibliométrico sobre Cadernos de Laboratório Eletrónicos

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22.11.2024

11.º FÓRUM
GESTÃO DE DADOS
DE INVESTIGAÇÃO
21-22 DE NOVEMBRO 2024
INSTITUTO POLITÉCNICO DE VISEU

Motivação e Abordagem

- Compreender a evolução e perfil das publicações sobre ELNs
- Identificar publicações relevantes para a comunidade GDI

Amostra: 187 documentos

- Web of Science (WoS) – Clarivate
- Core Collection
- Electronic Lab* Notebook* (Topic)
- Article **OR** Review Article **OR** Proceeding Paper **OR** Book **OR** Chapters

Topic

Searches title, abstract, keyword plus, and author keywords.

Document Types

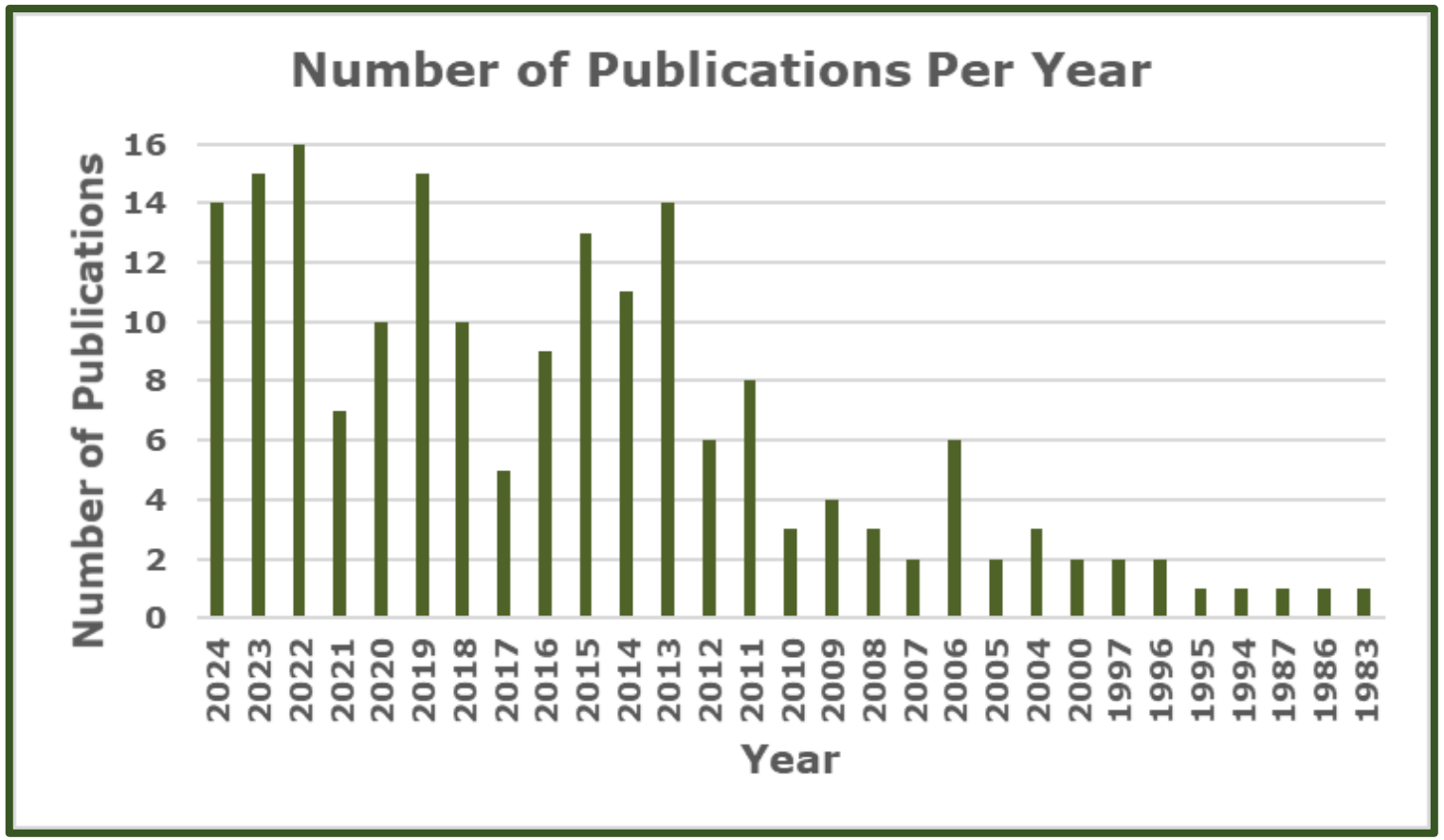
Article	143
Proceeding Paper	29
Review Article	19
Book Chapters	5

Languages

English	185
Japanese	1
Russian	1

Open Access

All Open Access	88
Gold	43
Gold-Hybrid	25
Free to Read	8
Green Published	42
Green Accepted	13
Green Submitted	21



Science Citation Index Expanded (SCI-EXPANDED)	144	Emerging Sources Citation Index (ESCI)	12	Book Citation Index – Science (BKCI-S)	5
Conference Proceedings Citation Index – Science (CPCI-S)	26	Conference Proceedings Citation Index – Social Science & Humanities (CPCI-SSH)	6	Social Sciences Citation Index (SSCI)	5

Publicação por Instituição

INSTITUIÇÃO	PAÍS	DOCUMENTOS
UNIVERSITY OF SOUTHAMPTON	INGLATERRA	15
HELMHOLTZ ASSOCIATION	ALEMANHA	12
PFIZER	EUA	10
ASTRAZENECA	INGLATERRA	9
KARLSRUHE INSTITUTE OF TECHNOLOGY	ALEMANHA	9
UNIVERSITY OF SYDNEY	AUSTRALIA	6
MERCK & COMPANY	EUA	5
BRISTOL-MYERS SQUIBB	EUA	5
UNIVERSITY OF CALIFORNIA SYSTEM	EUA	5
JANSEEN PHARMACEUTICALS	EUA	5

Publicação por País

PAÍS	DOCUMENTOS
ESTADOS UNIDOS DA AMÉRICA	75
ALEMANHA	46
REINO UNIDO	41
SUIÇA	12
JAPÃO	8
CANADÁ	8
FRANÇA	7
AUSTRALIA	7
SUÉCIA	7
PAÍSES BAIXOS	5

Publicação por Área de Investigação

Research Area	Web of Science Documents	Times Cited
1 Clinical & Life Sciences	84	882
2 Chemistry	46	1,135
6 Social Sciences	20	65
4 Electrical Engineering, Electronics & Computer Science	15	92
5 Physics	6	60
3 Agriculture, Environment & Ecology	3	16
7 Engineering & Materials Science	1	1
9 Mathematics	1	2

TÓPICOS - MESO	DOCUMENTOS
MEDICAL ETHICS	75
PROTEIN STRUCTURE, FOLDING & MODELLING	46
MOLECULAR & CELL BIOLOGY - GENETICS	41
EDUCATION & EDUCATIONAL RESEARCH	12
SOCIAL REFORM	8
CHROMATOGRAPHY & ELECTROPHORESIS	8
DISTRIBUTED & REAL TIME COMPUTING	7
MICROFLUIDIC DEVICES & SUPERHYDROPHOBICITY	7
MASS SPECTROMETRY	7
CHEMOMETRICS	5

Primeira Publicação Identificada

AN ELECTRONIC LABORATORY NOTEBOOK

By	FINMAN, J (FINMAN, J)
Source	AMERICAN LABORATORY Volume: 15 Issue: 2 Page: 98-&
Published	1983
Indexed	1983-01-01
Document Type	Article
Author Information	Corresponding Address: FINMAN, J (corresponding author) BBN RES SYST,10 MOULTON ST,CAMBRIDGE,MA 02238, USA Addresses : FINMAN, J; BBN RES SYST,10 MOULTON ST,CAMBRIDGE,MA 02238, USA:
Categories/ Classification	Research Areas: Chemistry; Instruments & Instrumentation Citation Topics: 2 Chemistry › 2.244 Chemometrics › 2.244.2183 Laboratory Systems
Web of Science Categories	Chemistry, Analytical; Instruments & Instrumentation
Language	English
Accession Number	WOS:A1983QD86300012
ISSN	0044-7749
IDS Number	QD863

Publicações com Autores Portugueses

EnzymeML: seamless data flow and modeling of enzymatic data

By Lauterbach, S (Lauterbach, Simone) [1] ; Dienhart, H (Dienhart, Hannah) [1] ; Range, J (Range, Jan) [1] ; Malzacher, S (Malzacher, Stephan) [2] , [3] ; Spöring, JD (Spoering, Jan-Dirk) [2] , [3] ; Rother, D (Rother, Doerte) [2] , [3] ; Pinto, MF (Pinto, Maria Filipa) [4] ; Martins, P (Martins, Pedro) [4] ; Lagerman, CE (Lagerman, Colton E.) [5] ; Bommarius, AS (Bommarius, Andreas S.) [5] ; Host, AV (Host, Amalie Vang) [6] ; Woodley, JM (Woodley, John M.) [6] ; Ngubane, S (Ngubane, Sandile) [7] ; Kudanga, T (Kudanga, Tukayi) [7] ; Bergmann, FT (Bergmann, Frank T.) [8] ; Rohwer, JM (Rohwer, Johann M.) [9] ; Iglezakis, D (Iglezakis, Dorothea) [10] ; Weidemann, A (Weidemann, Andreas) [11] ; Wittig, U (Wittig, Ulrike) [11] ; Kettner, C (Kettner, Carsten) [12] ; Swainston, N (Swainston, Neil) [13] ; Schnell, S (Schnell, Santiago) [14] ; Pleiss, J (Pleiss, Juergen) [1] ...Less

View Web of Science ResearcherID and ORCID (provided by Clarivate)

Source NATURE METHODS

Volume: 20 Issue: 3 Page: 400-+

DOI: 10.1038/s41592-022-01763-1

Published MAR 2023

Early Access FEB 2023

Indexed 2023-09-12

Document Type Article

Jump to ↓ Enriched Cited References

Abstract The design of biocatalytic reaction systems is highly complex owing to the dependency of the estimated kinetic parameters on the enzyme, the reaction conditions, and the modeling method. Consequently, reproducibility of enzymatic experiments and reusability of enzymatic data are challenging. We developed the XML-based markup language EnzymeML to enable storage and exchange of enzymatic data such as reaction conditions, the time course of the substrate and the product, kinetic parameters and the kinetic model, thus making enzymatic data findable, accessible, interoperable and reusable (FAIR). The feasibility and usefulness of the EnzymeML toolbox is demonstrated in six scenarios, for which data and metadata of different enzymatic reactions are collected and analyzed. EnzymeML serves as a seamless communication channel between experimental platforms, electronic lab notebooks, tools for modeling of enzyme kinetics, publication platforms and enzymatic reaction databases.

Grassroots Meets Grasstops: Integrated Research Data Management with EUDAT B2 Services, Dendro and LabTablet

da Silva, JR; Pereira, N; (...); Barros, B

22nd International Conference on Theory and Practice of Digital Libraries (TPDL)

2018 | DIGITAL LIBRARIES FOR OPEN KNOWLEDGE, TPDL 2018 11057 , pp.359-362

We present an integrated research data management (RDM) workflow that captures data from the moment of creation until its deposit. We integrated LabTablet, our electronic laboratory notebook, Dendro, our data organisation and description platform aimed at collaborative management of research data, and EUDAT's B2DROP and B2SHARE platforms. This approach combines the portability and automated metadata production abilities of LabTablet, Dendro as a collaborative RDM tool for dataset preparation, with the scalable storage of B2DROP and the long-term deposit of datasets in B2SHARE. The resulting workflow can be put to work in research groups where laboratorial or field work is central.

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Engaging Researchers in Data Management with LabTablet, an Electronic Laboratory Notebook

Amorim, RC; Castro, JA; (...); Ribeiro, C

4th International Symposium on Languages, Applications and Technologies (SLATE)

2015 | LANGUAGES, APPLICATIONS AND TECHNOLOGIES, SLATE 2015 563 , pp.216-223

Dealing with research data management can be a complex task, and recent guidelines prompt researchers to actively participate in this activity. Emergent research data platforms are proposing workflows to motivate researchers to take an active role in the management of their data. Other tools, such as electronic laboratory notebooks, can be embedded in the laboratory environment to ease the collection of valuable data and metadata as soon as it is available. This paper reports an extension of the previously developed LabTablet application to gather data and metadata for different research domains. Along with this extension, we present a case study from the social sciences, concerning the identification of the data description requirements for one of its domains. We argue that the LabTablet can be crucial to engage researchers in data organization and description. After starting the process, researchers can then manage their data in Dendro, a staging platform with stronger, collaborative management capabilities, which allows them to export their annotated datasets to selected research data repositories.

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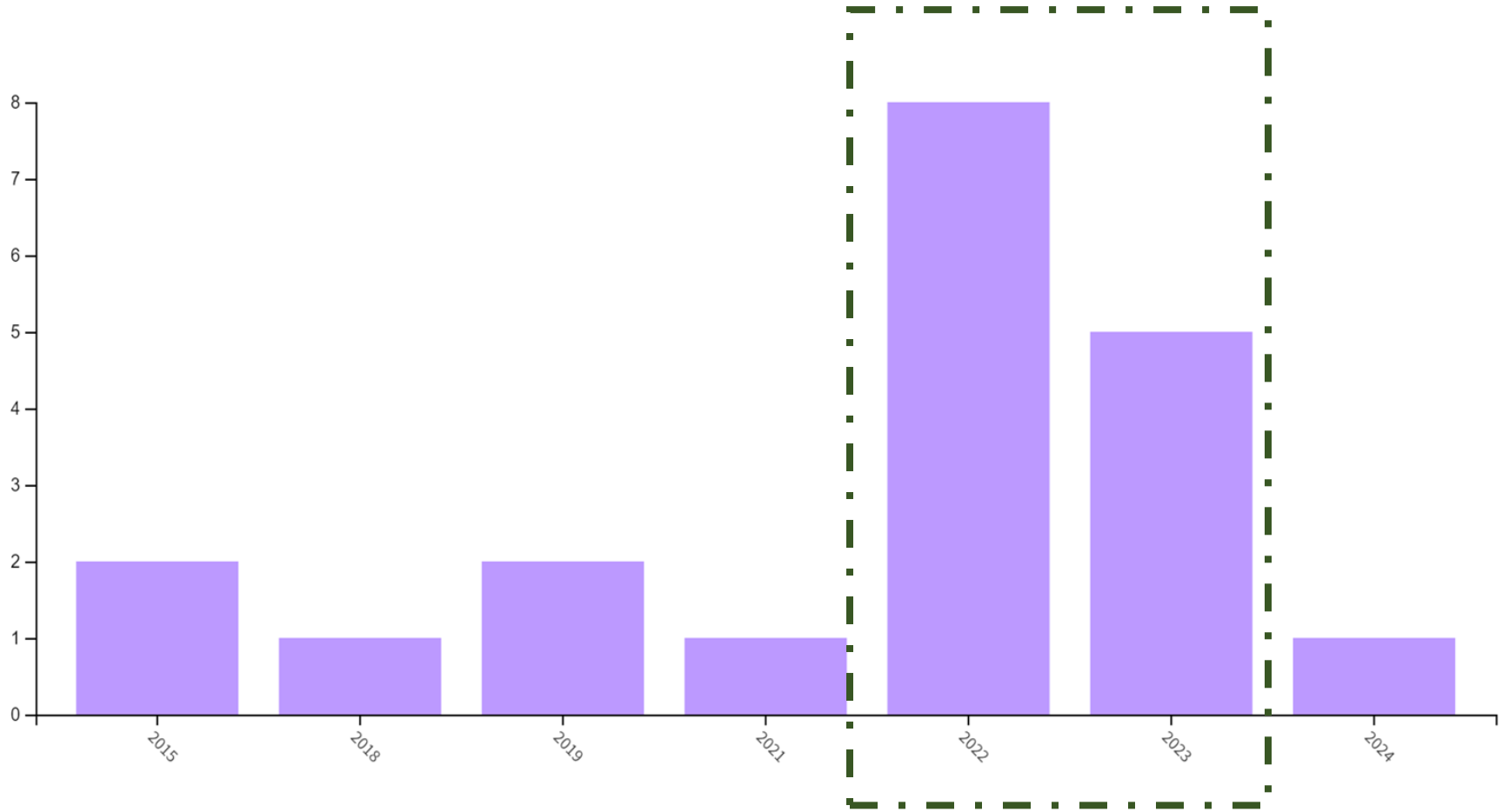
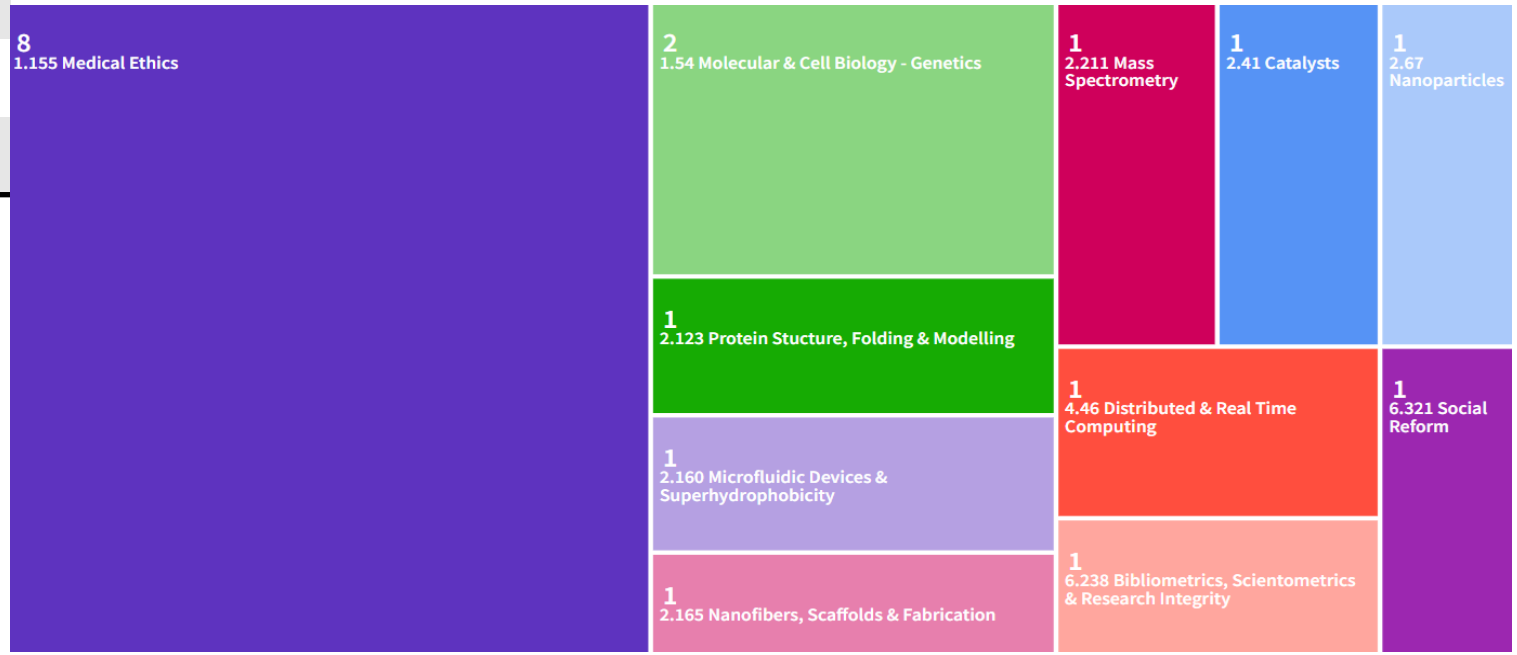
Bibliographic Database: Web of Science [WoS] – Clarivate
Collection: Web of Science Core Collection
Topic: "Research Data Management" AND "Electronic Lab* Notebook*"
Type of Docs: Article OR Review Article OR Proceeding Paper OR Book OR Chapters
Number of Documents: 20



ELN + GDI
(País e Área de Investigação)

PAÍS	DOCS
ALEMANHA	13
ESTADOS UNIDOS DA AMÉRICA	4
PORTUGAL	2
INGLATERRA	1
COREIA DO SUL	1



Identificação de artigos relevantes para a comunidade GDI

1 FAIR Data and Software: Improving Efficiency and Quality of Biocatalytic Science

Pleiss, J

Feb 7 2024 | ACS CATALYSIS 14 (4) , pp.2709-2718

Biocatalysis is entering a promising era as a data-driven science. High-throughput experimentation generates a rapidly increasing stream of biocatalytic data, which is the raw material for mechanistic and data-driven modeling to design improved biocatalysts and bioprocesses. However, our laboratory routines and our scientific practice of communicating scientific results are insufficient to ensure the reproducibility and scalability of experiments, and data management has become a bottleneck to progress in biocatalysis. In order to take full advantage of rapid progress in experimental and computational technologies, biocatalytic data should be findable, accessible, interoperable, and reusable (FAIR). FAIRification of data and software is achieved by developing standardized data exchange formats and ontologies, by electronic lab notebooks for data acquisition and documentation of experimentation, collaborative platforms for developing software and analyzing data, and repositories for publishing results together with raw data. The EnzymeML platform provides reusable and extensible tools and formats for FAIR and scalable data management in biocatalysis. FAIRification of data and software and the digitalization of biocatalysis are expected to improve the efficiency of research by automation and to guarantee the quality of biocatalytic science by reproducibility. Most of all, they foster reasoning and creating hypotheses by enabling the reanalysis of previously published data, and thus promote disruptive research and innovation.

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2 Results of a Three-Year Survey on the Implementation of Research Data Management and the Electronic Laboratory Notebook (ELN) Chemotion in an Advanced Inorganic Lab Course

Fink, F; Hoffmann, A and Herres-Pawlis, S

Oct 12 2023 | JOURNAL OF CHEMICAL EDUCATION 100 (11) , pp.4287-4297

As ongoing digitalization accelerates the execution of experiments and the documentation and storage of the corresponding data substantially, appropriate research data management (RDM) is a necessity to enable sustainable research at all. Consequently, a rethinking is currently taking place in academia. This process becomes visible by the utilization of electronic laboratory notebooks (ELNs) for documentation, the publication of research data in repositories, or the publishers' requirement for authors to provide a data availability statement. Despite the growing awareness of RDM in academia, the integration of the topic into curricula of chemistry studies is, if at all, in its infancy. As an initial example of incorporating RDM into curricula, an ELN was implemented in an advanced inorganic lab course for upper-division undergraduate students three years ago, supported by learning materials on RDM in general. A survey among the students helped, first, tracking the implementation of the ELN and the integration of RDM and, second, improving teaching materials and concepts. The three-year follow-up shows a growing awareness of RDM and higher acceptance toward ELNs among the students. The survey results highlight the need for and progress in teaching RDM in an early stage of chemistry studies already. Moreover, the possibility to integrate the topic here as a hands-on experience is a facile method for fast integration into teaching without changing the complete curricula.

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3 LISTER: Semiautomatic Metadata Extraction fr Annotated Experiment Documentation in eLabFTW

Musyaffa, FA; Rapp, K and Gohlke, H

Sep 29 2023 | JOURNAL OF CHEMICAL INFORMATION AND MODELING 63 (20) , pp.6224-6238

Enriched Cited References

The availability of scientific methods, code, and data is key for reproducing an experiment. Research data should be made available following the FAIR principle (findable, accessible, interoperable, and reusable). For that, the annotation of research data with metadata is central. However, existing research data management workflows often require that metadata be created by the corresponding researchers, which takes effort and time. Here, we developed LISTER as a methodological and algorithmic solution to create and extract metadata from annotated, template-based experimental documentation using minimum effort. We focused on tailoring the integration between existing platforms by using eLabFTW as the electronic lab notebook and adopting the ISA (investigation, study, assay) model as the abstract data model framework. LISTER consists of four components: annotation language to support metadata extraction; customized eLabFTW entries using specific hierarchies, templates, and tags to structure reusable scientific documentation; a "container" concept in eLabFTW, making metadata of a particular container content extractable along with its underlying, related experiments via a single click; a Python-based app to enable easy-to-use, semiautomated metadata extraction from eLabFTW entries. LISTER outputs metadata in machine-readable .json and human-readable .xlsx formats, and Material and Methods (MM) descriptions in .docx format that could be used in a thesis or manuscript. The metadata can be used as a basis to create or extend ontologies, which, when applied to the published research data, will significantly enhance its value. DSpace is used as a data cataloging platform for hosting the extracted metadata and research data. We applied LISTER to computational biophysical chemistry, protein biochemistry, and molecular biology, and our concept should be extendable to other life science areas.

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4 The Impact of Digitalized Data Management on Materials Systems Workflows

Tristram, F; Jung, N; (...); Bröse, S

May 2024 | ADVANCED FUNCTIONAL MATERIALS 34 (20)

The basic modules for materials research are systems for the design, synthesis, preparation, analysis, and application of materials and materials systems. To be efficient and produce findable, accessible, interoperable, and reusable (FAIR) data, state-of-the-art materials research needs to consider the integration of research data management (RDM) workflows and, in the end, the implementation of process automation concepts for all parts of the main modules. Here, the state-of-the-art methods of RDM in academia are described and a perspective on the future of digitalized molecular material systems workflows is given. The different elements of an integrated research data management strategy are described, and examples of automated processes are depicted. As such, the use of electronic lab notebooks for comprehensive documentation, the use of data-integration and data-conversion strategies, and the establishment of two platforms that enable the automated synthesis of chemical components for materials and the analysis of materials by electron microscopy, are highlighted. Two examples of beneficial effects of successful RDM strategies are presented, showing a sophisticated tool for data prediction based on machine learning and options for creating community-driven databases by extracting and re-using data from different scientific projects.

The discovery of the recent advancements in research data management (RDM) for materials research, including streamlined workflows, findable, accessible, interoperable, and reusable data, and automation are reported. From electronic lab notebooks to data conversion strategies, the benefits of state-of-the-art RDM are detailed. With machine learning predictions and community-driven databases, digitization is reshaping research on molecular material systems. image

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5 Needs assessment towards research data management at the Medical Faculty of the University of Freiburg-Data of the BE-KONFORM study

Fichtner, UA; Horstmeier, LM; (...); Knaus, J

Jun 2023 | DATA IN BRIEF 48

In order to investigate employees' needs of the Medical Faculty of the University of Freiburg regarding research data management, the BE-KONFORM study was performed in a two-step approach. First, guideline-based qualitative video interviews with four researchers were performed to identify key constructs of relevance. Second, a standardized online survey was conducted from 1 (st) to 15(th) of November 2020 based on e-mail invitation by the dean and a faculty newsletter. The questionnaire was provided bilingual (English and German) using a backward-forward translation method, no reminders and incentives were used to increase the response rate. The online survey was programmed in REDCap and was accessible via online link. The target population were members of the Medical Faculty (listed in the newsletter mailing list) regardless of the type of working contract signed. The final dataset contains 236 complete cases (90% German and 10% English). The study includes a randomised module asking for data publication (group A) or not (group B). 113 cases were randomized into group A and 99% of them consented to the publication of the collected research data in anonymized form (n = 112). The dataset comprised questions about work-related characteristics (professional status, working experience, scientific field of work), data management-related items (definition of research data management, type of data used, type of storage used for saving data, use of electronic laboratory notebooks), experience and attitudes towards data publication in data repositories, as well as needs and preferences regarding research data management support. The produced data offers the possibility to connect with other data collected in this field in other contexts (faculties or universities). (c) 2023 The Author(s). Published by Elsevier Inc. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/)

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6 Leveraging socio-technical processes to support researchers

Smith, P

Jul 26 2023 | DIGITAL LIBRARY PERSPECTIVES 39 (3) , pp.267-292

Purpose- The purpose of this project was to develop research support services that address local and external research data management (RDM) support drivers within the existing organizational culture at the University of Florida. The goal was to prompt organization change to support a campus-wide electronic lab notebook.Design/methodology/approach- This project used a mixed-methods research approach to cultivate an organizational change program that support technological infrastructure to benefit researchers. The mixed-methods research involved participation action research integrated with a stakeholder approach.Findings- The development of the grant proposal which was unfunded led to development of continued project goals. This project confirmed the development for support for an institution-wide electronic research notebook (ERN) solution requires adherence to the summary of five key actions for developing RDM services. Failure to complete all of the key actions engenders fragmentation culture.Research limitations/implications- This project includes implications for institutions to develop grant proposals with integrated budgets for research support services of funded projects; and to use the summary of key actions for developing RDM services articulated by Jones et al. (2013) in "How to Develop RDM Services - a guide for HEIs." Both are need to support findable, accessible, interoperable and reusable data for researchers.Practical implications- This project has practical implications for higher education institutions interested in leveraging socio-technical processes to advance the role of libraries as collaborator, partner and stakeholder in developing institution-wide adoption, support and training for ERN as a research support service to RDM.Social implications- This paper contributes to the body of developing literature on ERN as support services to RDM lead by academic research libraries.Originality/value- This project contributed to the change in organization culture resulting in the successful collaboration between the Research Office and College of Medicine to support an institution-wide ERN technological infrastructure for one year as a pilot at a large academic research institution in the southeast USA.

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7 Sharing is Caring: Guidelines for Sharing in the Electronic Laboratory Notebook (ELN) Chemotion as applied by a Synthesis-oriented Working Group

Fink, F; Hüppe, HM; (...); Herres-Pawlis, S

Oct 2022 | CHEMISTRYMETHODS 2 (10)

The documentation and storage of experimental data is crucial in research data management and science in general. With regard to automated data curation and the generation of data for machine learning processes, the collection and sharing of machine-readable data, including negative results, is a key step. The electronic laboratory notebook (ELN) Chemotion provides the possibility to share synthesis data with other scientists taking the mentioned aspects into account. In these guidelines, we offer general information on how to share data in Chemotion and present our sharing policy as a best practice example on how to use Chemotion's sharing functions in a working group with several group members on various hierarchy levels.

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8 A New Approach to Research Data Management with a Focus on Traceability: Adacta

Gossler, H; Riedel, J; (...); Deutschmann, O

Nov 2022 | CHEMIE INGENIEUR TECHNIK 94 (11) , pp.1798-1807

Enriched Cited References

Traceability between samples, devices and data is of great importance to the catalysis community. Adacta is a new research data management (RDM) system designed to create a traceable digital twin of a testing environment, not only storing data, but also creating a readily retrievable time-accurate record of the critical components used to measure catalyst performance. Future developments include extending Adacta to interact with electronic laboratory notebooks and to spawn simulations directly using data and measurements stored in the database.

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9 Structured Data Storage for Data-Driven Process Optimisation in Bioprinting

Schmieg, B; Brandt, N; (...); Hubbuch, J

Aug 2022 | APPLIED SCIENCES-BASEL 12 (15)

Bioprinting is a method to fabricate 3D models that mimic tissue. Future fields of application might be in pharmaceutical or medical context. As the number of applicants might vary between only one patient to manufacturing tissue for high-throughput drug screening, designing a process will necessitate a high degree of flexibility, robustness, as well as comprehensive monitoring. To enable quality by design process optimisation for future application, establishing systematic data storage routines suitable for automated analytical tools is highly desirable as a first step. This manuscript introduces a workflow for process design, documentation within an electronic lab notebook and monitoring to supervise the product quality over time or at different locations. Lab notes, analytical data and corresponding metadata are stored in a systematic hierarchy within the research data infrastructure Kadi4Mat, which allows for continuous, flexible data structuring and access management. To support the experimental and analytical workflow, additional features were implemented to enhance and build upon the functionality provided by Kadi4Mat, including browser-based file previews and a Python tool for the combined filtering and extraction of data. The structured research data management with Kadi4Mat enables retrospective data grouping and usage by process analytical technology tools connecting individual analysis software to machine-readable data exchange formats.

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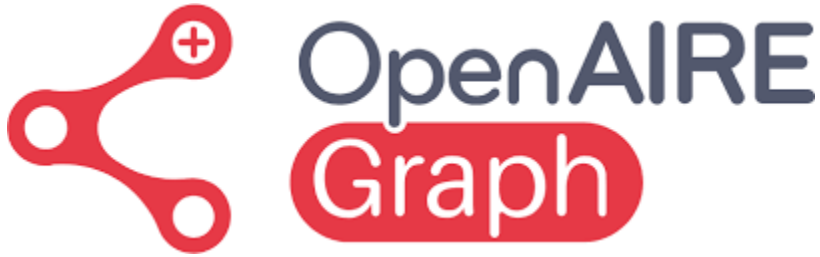
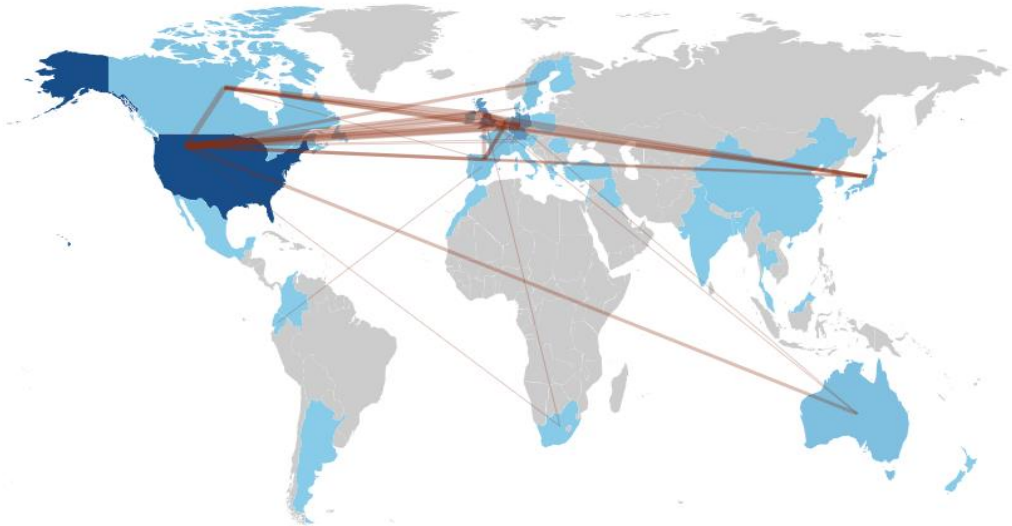
Direções futuras

Ampliação do estudo para abranger outras fontes de informação bibliométrica abertas

Necessidade de curadoria de metadados e integração com as bases de dados tradicionais



Conclusão

- Revistas no domínio da Química são as que mais publicam sobre ELNs.
  (Chemical Information and Modeling | Chemical Education | ChemoInformatics)
- Trabalho em desenvolvimento - **Melhoria contínua do processo e curadoria da amostra.**
- Recursos a partilhar com a Comunidade GDI - **Dataset e lista curada de publicações relevantes.**

14% dos artigos em Cooperação Internacional