

Special Collection

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

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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.

Introduction

The digital revolution is transforming chemistry in an unprecedented way: computational chemistry allows the detailed description of reaction mechanisms,^[1] methods of machine learning enable retrosynthesis and the prediction of material properties,^[2,3] and software designed to control chemical reaction processes, such as a Chemputer to perform syntheses and their optimization in automated feedback-loops.^[4,5]

While analytical data are already mainly generated and stored digitally, many scientists still use handwritten laboratory notebooks to record the experiments related to their obtained analytical data.^[6–8] Recording experiments in an analogous way leads to several disadvantages, like limited accessibility for scientists outside the laboratory, possible misinterpretation due to illegibility, or the missing connection to the digitally stored data. Thus, reasonable data management and sustainable research is only hardly feasible.^[9]

In the long run, chemical databases will probably allow to map the chemical reaction space to teach artificial intelligence

to understand the laws of chemistry.^[10–12] Therefore, not only positive results but also negative ones need to be reported in a systematic way.^[13,14]

Fortunately, the way experiments are recorded in chemistry and its related sciences is changing. In the recent years, many electronic laboratory notebooks (ELNs) were developed providing solutions to document and store experiments in a systematic manner.^[15,16] There are many generic ELNs, like LabFolder,^[17] RSpace,^[18] or eLabFTW^[19,20] but also specific systems for chemistry^[21,22] exist which support essential needs such as the processing of chemical structures,^[23] thus making the reactions and obtained molecules machine-readable. Examples for such chemistry-specific ELNs which are available as an open source are LabTrove,^[24–26] Indigo ELN,^[27,28] and Open Enventory.^[29–31]

A highly useful and sustainable open source option for recording and managing experiments and data in chemistry is Chemotion.^[32] Chemotion consists of two major systems: the electronic lab notebook Chemotion ELN^[33] to record and manage research data and Chemotion repository which is used to publish research data.^[34,35] The data from the ELN can easily be transferred into the repository and then published as a data publication. After publication in the Chemotion repository, these datasets, also including analytic raw data in a non-proprietary data format, receive a unique digital object identifier (DOI)^[36] and are accessible to the whole scientific community under a Creative Commons license (CC0, CC BY or CC BY-SA license). Moreover, the deposited data then are synchronized to PubChem and Scifinder where they can easily be accessed.

Chemotion is developed, improved, extended, and promoted within the framework of the consortium NFDI4Chem (National Research Data Infrastructure for Chemistry, Germany).^[37,38] Here, the main goal is to offer Chemotion as a system which enables the digitalization in chemistry also for those scientists that cannot afford other systems. Further on, the consortium develops minimal information standards for data publications, such as standards for data and metadata

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formats and ontologies (controlled vocabularies) for semantic descriptions.^[39,40] Overall, NFDI4Chem aims to support digitalization in chemistry by providing a national infrastructure for research data management.^[41]

For reaching the goals of NFDI4Chem, the use of ELNs and repositories is the key step. Using the Chemotion ELN already for planning an experiment, facilitates research data management in general and compliance with the FAIR data principles (findable, accessible, interoperable, reusable)^[42] in particular. Publication of these research data in the Chemotion repository afterwards fulfills the FAIR data principles as well: published datasets are findable due to their unique DOI, are accessible and downloadable to scientists after registration in the repository for free, and are stored as interoperable file formats enabling their reuse.^[34,35] Thus, following the FAIR data principles is a key requirement for sharing research data with the scientific community in a sustainable manner.

However, managing and sharing research data always begins on a much smaller scale. Within a laboratory, working group, or institution data are exchanged day by day between colleagues, with students, apprentices, senior scientists in the group, supervisor(s), collaborators, or internal reviewers. Here, the Chemotion ELN provides a feature to share data easily with others on various hierarchy levels. Furthermore, the sharing feature of the ELN offers the possibility to generate shared databases, for example, for purchased chemicals, synthesized ligands, or already published experiments. These joint databases are a FAIR environment for data exchange within a laboratory, working group, institution microcosm, or even research centers, and thus represent on a much smaller scale an equivalent to the Chemotion repository's function for data exchange.

In this contribution we explain how to share data in the Chemotion ELN and present our Sharing Policy as a best practice example on how to use the sharing feature. Thus, we

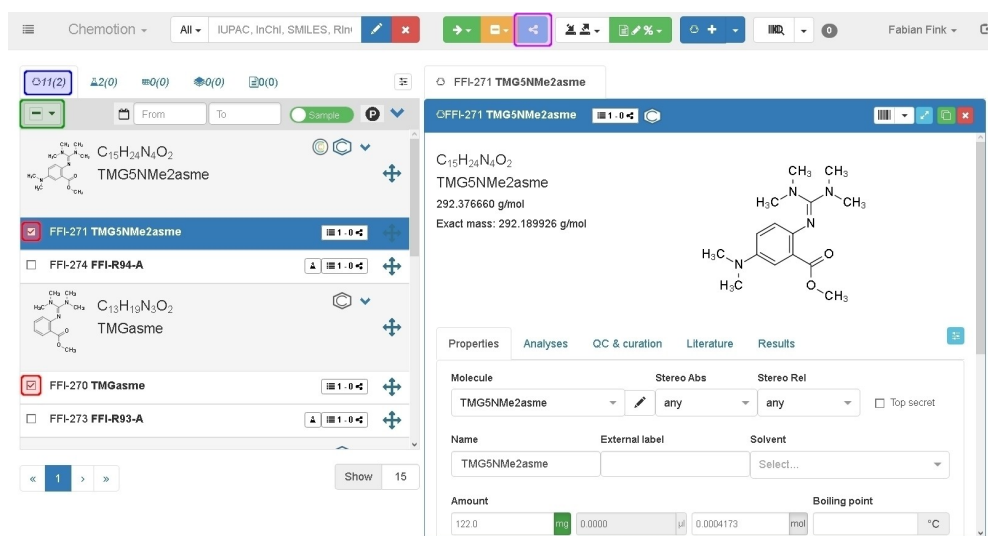
consider a basic knowledge about the usage of Chemotion as a requirement here, as we will not go into detail on basic operations. For basic information on the electronic lab notebook we recommend the documentation^[43] and explanatory videos.^[44]

Sharing Data

There are two different possibilities to share data in the electronic laboratory notebook Chemotion. First, a selection of specific elements (samples, reactions, wellplates, screens, research plans, or other entities) can be shared with others. Sharing selected elements results in sharing a snapshot of the dataset at the time the sharing was carried out. Subsequent additions to the datasets (e.g., in form of sharing additional entities such as additional reactions) are not intended, only changes to the existing shared data are applied and can be accessed by all users. Second, collections of data can be shared with other users. The sharing of collections results in the creation of a collection of data that can be extended after its creation. New entities, such as a new reaction, assigned to the existing shared collection, are synchronized with the already shared data and are accessible to others. Sharing collections enables a permanent adoption of data to diverse changes.

How to share data

To explain the sharing functions, we have chosen a ligand system from our research as an example. TMG₅Me₂asme and TMG₅NMe₂asme (molecular structure depicted in Figure 1) are guanidine ligands based on methyl anthranilate. We have chosen this example for two reasons: first, zinc complexes containing these ligands represent active catalysts in the ring-



The screenshot shows the Chemotion software interface. On the left, a list of samples is displayed with checkboxes and selection icons. A red box highlights the 'FFI-271 TMG5NMe2asme' entry, a green box highlights the selection icons, a blue box highlights the counter '1', and a purple box highlights the sharing icon. On the right, a detailed view of the molecule 'FFI-271 TMG5NMe2asme' is shown, including its chemical structure, molecular formula (C₁₅H₂₄N₄O₂), molar mass (292.376660 g/mol), and exact mass (292.189926 g/mol). The interface also shows various tabs like Properties, Analyses, QC & curation, Literature, and Results.

Figure 1. Picking of entities such as samples, reactions, wellplates, screens, and research plans from a collection to share (red box = picking of entries, green box = selecting/unselecting of all entries, blue box = counter for selected entries, purple box = sharing button to begin the sharing process). Here only shown for the tab "sample". Detail view of the molecule TMG₅NMe₂asme opened as example is shown on the right side.

opening polymerization (ROP) of lactide.^[45,46] However, the ligand system was passed to another PhD student via a joint database resulting in iron complexes which are even more active in the ROP^[47,48] and, additionally, promote the combination of the ROP of lactide with the atom transfer radical polymerization (ATRP) of styrene.^[49] Second, the ligand system was further modified in the backbone of the ligand.^[46] We generated a library of various catalysts for the ROP which can serve as datasets in machine learning processes. Thus, we can work on the understanding of the influence of ligand design and metal choice on the activity of the catalysts and predict further developments in the field.

To use the share function, all samples, reactions etc. to be shared were selected (red box, Figure 1). After selecting an entity, the counter in the open tab increases (value in the parentheses, blue box in Figure 1). It is possible to share entries from different tabs (samples, reactions, ...) simultaneously. The check box at the top (green box) offers the possibility to select/unselect all entries of the active page. After picking all desired entities clicking on the light blue sharing button at the top of the page starts the sharing process (purple box).

Upon clicking, a pop-up window opens up (Figure 2). Here, the sharing role, the permission level, the detail level, and the users to share with can be adjusted. The sharing role is optional and offers the following options: user, partner, collaborator, reviewer, or supervisor. Picking a sharing role leads to default settings for the permission and detail levels. For the permission

Figure 2. Pop-up window after clicking on the sharing button with the adjustment options for the sharing role, the permission level, the detail level, and the users to share with.

level the options read, write, share, delete, import elements, and pass ownership can be chosen. Higher permission levels include all possibilities of the lower ones, for example, applying the “delete” permission allows the user also to read, write, and share. Additionally, the detail level for each category of entries (sample, reaction, wellplate, and screen) can be adjusted separately. Finally, the users with whom the data are shared have to be selected. Data can be shared with a single person, several people, or whole groups. Groups have to be created in the settings of Chemotion under “My Groups” before they can be used for the sharing option. Here, it is important that all users have a Chemotion account on the same instance.

The shared collection is created by clicking on “Create Shared Collection” (Figure 2). In the taskbar on the left a new collection appears in “My shared collections” (red box, Figure 3). The collections in “My shared collections” are sorted by the user who shared the data and they are labeled with the users’ short labels. The shared elements are assigned to an additional management panel labeled “My Shared collections”. For the user who has access to the new shared entries, exactly the same collections are visible as “Shared with me” (blue box, Figure 3).

The sharing of selected items of the ELN which may also come from different collections is only one option to share data. For other purposes, the sharing of an existing collection is the right process. Sharing of collections can be defined in the collection management part of the ELN (blue box, Figure 4). In the tab “My Collections” the collection to be shared can be chosen by clicking on the blue sharing button (red box,

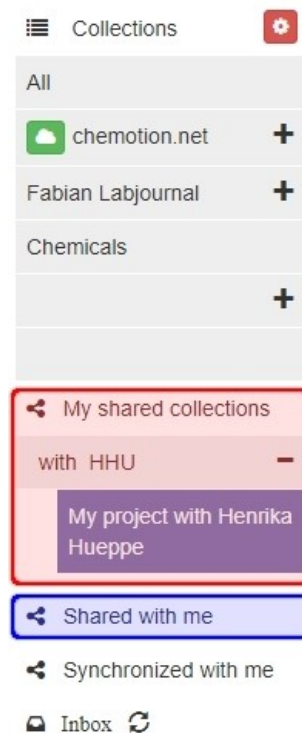


Figure 3. Overview on “My shared collections” with the subfolder structure (red box = “My shared collections”, blue box = “Shared with me”).

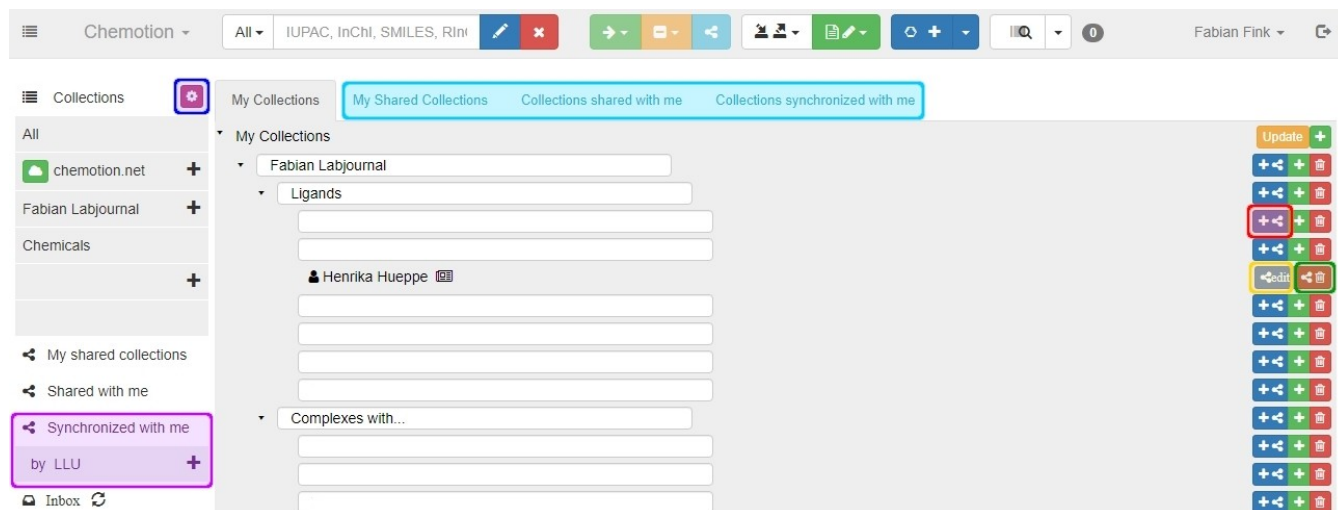


Figure 4. Picking collections on the settings page to synchronize and editing of synchronized and shared collections (blue box = collection button, red box = synchronizing button, purple box = “Synchronized with me”, yellow box = “Edit synchronized collection”, green box = “Delete synchronized collections”, light blue box = tabs for shared and synchronized collections).

Figure 4). A pop-up window opens up, offering the same adjustment options (role, permission and detail level, and users to share with) as described for the share function for individually selected entities (see Figure 2). After selecting the desired options, the shared collection is created by clicking on “Create Sync Shared Collection”.

Collections synchronized with other users are not shown in the taskbar on the left as an additional item. As these collections exist already, the original collection is labeled with a shared symbol to allow an easy visibility to the user. The users to whom the collection is shared see the shared item in their “Synchronized with me” list (purple box, Figure 4). To edit the options of the shared collections or to withdraw the sharing, the “Edit synchronized collection” button (yellow box, Figure 4) or the “Delete synchronized collection” button (green box, Figure 4) in the “My Collections” tab of the management collection section has to be chosen. Editing leads to the pop-up window (Figure 2) with the current configuration settings.

To edit or delete shared collections or collections that are shared by other users, the respective tab on the collection management page (light blue box, Figure 4) must be opened. Here, the options for editing and deleting are the same as mentioned in the last paragraph.

Sharing with collaborators on different permission levels

In this chapter, we describe the Sharing Policy as applied by the Herres-Pawlis’ working group as a best practice example. At the moment eighteen PhD students and five postdocs are members of the working group. In addition, there is a fluctuating number of trainees, research assistants, master, internship, and bachelor students; on average one to two times the number of PhD students. All team members are divided among approximately ten different subject areas.

Since the beginning of 2020, the working group uses Chemotion as an ELN to record experiments. Here, data are mainly shared between PhD students and their supervised students. Additionally, ELN entries are usually shared with senior supervisors for confirmation of the datasets and even external collaborators. In these two years 1270 reactions have been created and more than 7000 samples described. This is a large number taking into account that the working group transition to the ELN is a process which started in 2020 and which will be finished in 2022.

Depending on the person that shares data and with whom, the permission and detail level of datasets have to be adjusted accordingly. As the working group consists of many group members on various hierarchy levels working in different research fields, the establishment of a consistent and easily applicable sharing policy was needed. The resulting guidelines are described in the following chapters to give an overview of recommended permission and detail settings for sharing with different collaborators.

Table 1 shows all recommendations for the permission level to give a concise overview. The recommendations are stated as follows: each entry in the table comprises six different pictograms for the six different levels of permission (Figure 5). These levels are “Read”, “Write”, “Share”, “Delete”, “Import Elements”, and “Pass ownership” (from left to right in the figure). Permission levels that should be applied are colored green



Figure 5. Pictograms of the different levels of permission (from left to right: read, write, share, delete, import elements, and pass ownership). Permission levels that should be applied are colored green, levels that might be applied optionally are colored yellow, and levels that should not be applied are colored red.

Table 1. Overview of the recommended permission settings for sharing with different collaborators as realized in the Herres-Pawlis group (the permission level is visualized with the six different pictograms for the six different levels of permission and a traffic light color scheme as explained in Figure 5).

Shared by	Supervisor (or subgroup leader/postdoc)	PhD student (postdocs)	Master student	Internship student	Bachelor student	Trainee	External collaborator
Shared with							
Supervisor (or subgroup leader/postdoc)							External policies ^[b]
PhD student (postdocs)							External policies ^[b]
Master student							External policies ^[b]
Internship student							External policies ^[b]
Bachelor student							External policies ^[b]
Trainee							External policies ^[b]
External collaborator							External policies ^[b]

[a] Usually not necessary, ask the direct supervisor if needed, [b] Depends on the sharing policy of the collaborator.

(e.g., “Read” in Figure 5), levels that might be applied optionally are colored yellow (e.g., every level until “Import Elements”), and levels that should not be applied are colored red (e.g., “Pass ownership”).

Shared by trainees, bachelor, and internship students

Trainee, bachelor, or internship students should supply their direct supervisor (in this case a PhD student, postdoc, or subgroup leader) with the full detail level of the shared elements and entries. The “Read” permission should be used if the supervisor just needs to confirm datasets during the research or thesis. After completion of the research or thesis, the supervising scientist should receive at least an “Import Elements” permission to add the generated entries to their own ELN. The supervisor may also receive the “Pass ownership” permission. By using the permission level “Pass ownership” the option to take over elements and collections permanently is enabled for the user data are shared with. In the taskbar on the left, the user can then assign collections to the folder “Shared with me” or “Synchronized with me” (purple box, Figure 4) with a single click. Thus, the elements and collections are removed from one’s ELN and are integrated into the ELN of the other user.

If datasets have to be shared with a senior supervisor (subgroup leader, professor, or an internal peer reviewer) before publication in the Chemotion Repository,^[34,35] the “Read” permission on the highest detail level should be applied to enable confirmation of the data. Sharing data with master students, other trainees, bachelor, and internship students, or external collaborators is usually not necessary. If it is required, the direct supervisor should be asked how permission and detail level have to be adjusted.

Shared by master students

As a master student, sharing data with other active scientists (PhD students; postdocs; other master students; or trainee, bachelor, or internship students) depends on the further use of the data. If other scientists need the data only as a reference or to write a report, for example, their studies are based on the datasets provided, a simple “Read” permission should be sufficient. However, if synthesized compounds are used in further experiments by other scientists, they should have an “Import Elements” permission to add the compounds to their own ELN, for example to be used as a starting material. The “Import Elements” permission level also allows to delete shared elements. This should be pointed out to other scientists to prevent undesired deletion. Concerning the detail level, datasets should always be provided with the full detail level to avoid misunderstanding and misinterpretation of the data. The “Pass ownership” permission should never be used for sharing information with other scientists that are not supervisors.

For master students, the direct supervisor is usually a senior supervisor of the working group or the subproject (postdoc, subgroup leader, or professor). The recommendations for the detail and permission levels are similar to those for trainee, bachelor, and internship students and their direct supervisors, as mentioned in the last section. When a master student leaves the working group after the master thesis and does not continue with a PhD, the supervisor may also receive the “Pass ownership” permission.

Shared by PhD students

As a PhD student, the permission and detail levels for sharing data with other active scientists is the same as for master students, as stated in the last section. In addition, the

recommendations for sharing with the direct supervisor (in this case most likely the leader of the working group) are identical to those for master students.

Shared with external collaborators

When sharing data with external collaborators some difficulties may arise. It has to be considered that external groups or collaborators from industry might have a differing sharing policy. Moreover, an embargo might be placed on specific dataset or information concerning the research especially when working with collaborators from industry. Thus, the sharing of data might not be allowed. Possible arising issues concerning data and data sharing should be clarified in advance.

Here, the recommendations for permission and detail level are the same for all sharing parties (supervisors, PhD students, and master students): as much detail on the datasets as is necessary for the external collaborator to understand and interpret the data correctly should be provided. Usually, the “Read” permission level should be sufficient. A permission level up to “Import Elements” might be applied, if the collaborator uses the elements for further experiments or investigations. The ownership of ELN entries and datasets should never be passed to external collaborators.

Sharing data with Chemotion users working on another instance of Chemotion at another site/university is not possible if the ELN is set up within the protected environment of a university. Only if the ELN is installed outside the protected environment (as a publicly accessible instance), the sharing of data with external scientists is applicable. Technically, the exchange of information between different Chemotion instances can be achieved by exporting collections from one’s own Chemotion ELN account and then the data can be imported into the Chemotion ELN instance of other collaborators. As an alternative the Chemotion Repository^[34,35] is mentioned briefly. Here, datasets from the ELN can easily be transferred and published as a data publication with its own persistent identifier (PID). External collaborators can access the data on full detail level without having a Chemotion account on the same server or instance, then.

Shared by supervisors

A senior supervisor (postdoc, subgroup leader, or professor) should be able to supply all staff members (postdocs; PhD, master, internship, and bachelor students; or trainees) with data from previous years, projects, and students if required. Therefore, a permission level up to “Import Elements”, depending on the specific case, should be applied with the highest detail level to avoid misinterpretation, misunderstanding, and a lack of information. The “Pass ownership” permission should not be used.

A supervisor also functions as an internal peer reviewer of datasets before these are published, for example, in the Chemotion Repository. Thus, active scientists should provide

ELN entries to supervisors applying a “Read” permission on full detail level for confirmation of the accuracy of the data.

Joint databases

Creating a shared collection with all scientists of a laboratory, working group, or institution offers the possibility of joint databases. Especially in large working groups, institutions, or collaborative research centers, joint databases represent a powerful tool and can function as an internal repository. The databases offer a concise overview of ongoing and past work and allow scientists to share ideas or re-use information of others and to interconnect with scientists. Furthermore, the experimental data including also negative results and their corresponding metadata are machine-readable and can be applied in machine learning processes.

With regard to these joint databases, for example, for synthesized ligands, complexes, precursors, or catalysts, active scientists should enter their experiments and datasets on a regular basis. Therefore, datasets should be confirmed by a supervisor before a copy of the ELN entry on full detail level is added to the joint database to prevent unintentional deletion of the data by other users of the database.

Conclusion

Digitalization is a challenging process in chemistry and its related sciences and needs to be supported by software and infrastructure as the use of electronic laboratory notebooks (ELNs) and the establishment of data repositories. While ELNs enable the documentation, management, and storage of research data in a FAIR (findable, accessible, interoperable, reusable) manner repositories are used for the sharing of research data with the community. Repositories therefore have a crucial role to allow to exchange data between scientists sustainably and unrestrictedly. Nevertheless, data sharing is also relevant at a prior stage in the research data live cycle of data. ELNs, being often considered as tool for documentation only, can serve as a highly beneficial tool to enable the sharing of information on a much smaller scale between colleagues within laboratories, working groups, or institutions.

The ELN Chemotion provides functions to exchange data with others on various hierarchy levels. Such options are a prerequisite for the establishment of shared data but it needs also the agreement of scientists to a sharing policy. We propose herein such a policy as a best practice model to have a consistent and easily applicable guideline for all scientists in a working group. These guidelines may provide a foundation and recommendation for other laboratories, working groups, and institutions. As a result, sharing information follows concrete rules and a trustable environment is created for those scientists who work with digital tools. Scientists can share data to enable internal reviewing and feedback, they can support others with information on their work and can build joint databases within an environment for almost every desirable need: a Chemotion

collection shared with all researchers may function as a lab inventory for purchased chemicals, a database for specific subjects, or an internal repository for knowledge exchange between staff member generations.

Author Contributions

F.F., H.M.H. and S.H.-P. conceived the Sharing Policy, F.F. wrote the draft of the Sharing Policy, N.J. provided assistance with the functions of Chemotion, H.M.H., A.H., N.J. and S.H.-P. reviewed the Sharing Policy, F.F. wrote the original manuscript, all authors reviewed the manuscript.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

Keywords: Chemotion · data exchange · electronic laboratory notebook (ELN) · FAIR data · sharing policy

- [1] M. Foscatto, V. R. Jensen, *ACS Catal.* **2020**, *10*, 2354–2377.
- [2] J. A. Selekman, J. Qiu, K. Tran, J. Stevens, V. Rosso, E. Simmons, Y. Xiao, J. Janey, *Annu. Rev. Chem. Biomol. Eng.* **2017**, *8*, 525–547.
- [3] S. M. Mennen, C. Alhambra, C. L. Allen, M. Barberis, S. Berritt, T. A. Brandt, A. D. Campbell, J. Castañón, A. H. Cherney, M. Christensen, D. B. Damon, J. Eugenio de Diego, S. García-Cerrada, P. García-Losada, R. Haro, J. Janey, D. C. Leitch, L. Li, F. Liu, P. C. Lobben, D. W. C. MacMillan, J. Magano, E. McInturff, S. Monfette, R. J. Post, D. Schultz, B. J. Sitter, J. M. Stevens, I. I. Strambeanu, J. Twilton, K. Wang, M. A. Zajac, *Org. Process Res. Dev.* **2019**, *23*, 1213–1242.
- [4] D. Caramelli, J. M. Granda, S. H. M. Mehr, D. Cambié, A. B. Henson, L. Cronin, *ACS Cent. Sci.* **2021**, *7*, 1821–1830.
- [5] A. J. S. Hammer, A. I. Leonov, N. L. Bell, L. Cronin, *JACS Au* **2021**, *1*, 1572–1587.
- [6] O. Koepler, J. Liermann, F. Schön, S. Herres-Pawlis, *Nachr. Chem.* **2020**, *68*, 20–23.
- [7] S. Herres-Pawlis, J. C. Liermann, O. Koepler, *Z. Anorg. Allg. Chem.* **2020**, *646*, 1748–1757.
- [8] S. Herres-Pawlis, O. Koepler, J. C. Liermann, Dataset: First NFDI4Chem User Survey. **2020**, <https://doi.org/10.25835/0077933>.
- [9] Deutsche Forschungsgemeinschaft. *Guidelines for Safeguarding Good Research Practice. Code of Conduct.* **2019**, <https://doi.org/10.5281/zenodo.3923602>.
- [10] J.-L. Reymond, L. Ruddigkeit, L. Blum, R. van Deursen, *WIREs Comput. Mol. Sci.* **2012**, *2*, 717–733.
- [11] S. M. Kearnes, M. R. Maser, M. Wlekinski, A. Kast, A. G. Doyle, S. D. Dreher, J. M. Hawkins, K. F. Jensen, C. W. Coley, *J. Am. Chem. Soc.* **2021**, *143*, 18820–18826.
- [12] J. P. Janet, A. Tomberg, J. Boström, *Nat. Mach. Intell.* **2021**, *3*, 572–575.
- [13] P. Raccuglia, K. C. Elbert, P. D. F. Adler, C. Falk, M. B. Wenny, A. Mollo, M. Zeller, S. A. Friedler, J. Schrier, A. J. Norquist, *Nature* **2016**, *533*, 73–76.
- [14] M.-E. Herbet, J. Leonard, M. G. Santangelo, L. Albaret, *Learn. Publ.* **2022**, *35*, 16–29.
- [15] M. Rubacha, A. K. Rattan, S. C. Hosselet, *JALA* **2011**, *16*, 90–98.
- [16] B. Adam, B. Lindstädt *Elektronische Laborbücher im Kontext von Forschungsdatenmanagement und guter wissenschaftlicher Praxis - ein Wegweiser für die Lebenswissenschaften : ELN-Wegweiser.* **2020**, <https://doi.org/10.4126/FRL01-006422868>.
- [17] LabFolder. <https://www.labfolder.com/> (accessed 03/25/2022).
- [18] RSpace. <https://www.researchspace.com/> (accessed 03/25/2022).
- [19] eLabFTW. <https://www.elabftw.net/> (accessed 03/25/2022).
- [20] M. Hewera, D. Hanggi, B. Gerlach, U. D. Kahlert, *F1000Research* **2021**, *10*, 292.
- [21] K. T. Taylor, *Curr. Opin. Drug Discov. Devel.* **2006**, *9*, 348–353.
- [22] C. L. Bird, C. Willoughby, J. G. Frey, *Chem. Soc. Rev.* **2013**, *42*, 8157–8175.
- [23] S. J. Coles, J. G. Frey, C. L. Bird, R. J. Whitby, A. E. Day, *J. Cheminform.* **2013**, *5*, 52.
- [24] LabTrove. <https://labtrove.org/> (accessed 03/25/2022).
- [25] C. Willoughby, C. L. Bird, S. J. Coles, J. G. Frey, *J. Chem. Inf. Model.* **2014**, *54*, 3268–3283.
- [26] A. E. Day, S. J. Coles, C. L. Bird, J. G. Frey, R. J. Whitby, V. E. Tkachenko, A. J. Williams, *J. Chem. Inf. Model.* **2015**, *55*, 501–509.
- [27] Indigo ELN. <https://lifescience.opensource.epam.com/indigo/eln/index.html#> (accessed 03/25/2022).
- [28] Indigo, gga software. <https://github.com/ggasoftware/indigo> (accessed 03/25/2022).
- [29] Open Inventory. http://www.open-enventory.de/index_de.html (accessed 03/25/2022).
- [30] F. Rudolphi, L. J. Goossen, *Nachr. Chem.* **2010**, *58*, 548–550.
- [31] F. Rudolphi, L. J. Goossen, *J. Chem. Inf. Model.* **2012**, *52*, 293–301.
- [32] Chemotion. <https://chemotion.net/chemotionsaurus/> (accessed 03/25/2022).
- [33] P. Tremouilhac, A. Nguyen, Y.-C. Huang, S. Kotov, D. S. Lütjohann, F. Hübsch, N. Jung, S. Bräse, *J. Cheminform.* **2017**, *9*, 54.
- [34] P. Tremouilhac, C.-L. Lin, P.-C. Huang, Y.-C. Huang, A. Nguyen, N. Jung, F. Bach, R. Ulrich, B. Neumair, A. Streit, S. Bräse, *Angew. Chem. Int. Ed.* **2020**, *59*, 22771–22778; *Angew. Chem.* **2020**, *132*, 22960–22968.
- [35] P. Tremouilhac, P.-C. Huang, C.-L. Lin, Y.-C. Huang, A. Nguyen, N. Jung, F. Bach, S. Bräse, *Chemistry-Methods* **2021**, *1*, 8–11.
- [36] N. Paskin, *Interlend. Doc. Supply* **1999**, *27*, 13–16.
- [37] S. Herres-Pawlis, O. Koepler, C. Steinbeck, *Angew. Chem. Int. Ed.* **2019**, *58*, 10766–10768; *Angew. Chem.* **2019**, *131*, 10880–10882.
- [38] N. Jung, S. Neumann, O. Koepler, F. Bach, C. Popp, S. Herres-Pawlis, J. Liermann, M. Razum, C. Steinbeck, *Bunsen-Magazin* **2021**, 100–103.
- [39] J. Ortmeier, F. Schön, S. Herres-Pawlis, N. Jung, F. Bach, J. Liermann, S. Neumann, C. Popp, M. Razum, O. Koepler, C. Steinbeck, *Bausteine Forschungsdatenmanagement* **2021**, *2*, 34–45.
- [40] P. Strömert, J. Hunold, A. Castro, S. Neumann, O. Koepler, *Pure Appl. Chem.* **2022**, <https://doi.org/10.1515/pac-2021-2007>.
- [41] C. Steinbeck, O. Koepler, F. Bach, S. Herres-Pawlis, N. Jung, J. C. Liermann, S. Neumann, M. Razum, C. Baldauf, F. Biedermann, T. W. Bocklitz, F. Boehm, F. Broda, P. Czodrowski, T. Engel, M. G. Hicks, S. M. Kast, C. Kettner, W. Koch, G. Lanza, A. Link, R. A. Mata, W. E. Nagel, A. Porzel, N. Schlörer, T. Schulze, H.-G. Weinig, W. Wenzel, L. A. Wessjohann, S. Wulle, *Res. Ideas Outcomes* **2020**, *6*, e55852.
- [42] M. D. Wilkinson, M. Dumontier, I. J. Aalbersberg, G. Appleton, M. Axton, A. Baak, N. Blomberg, J.-W. Boiten, L. B. da Silva Santos, P. E. Bourne, J. Bouwman, A. J. Brookes, T. Clark, M. Crosas, I. Dillo, O. Dumon, S. Edmunds, C. T. Evelo, R. Finkers, A. Gonzalez-Beltran, A. J. G. Gray, P. Groth, C. Goble, J. S. Grethe, J. Heringa, P. A. C. 't Hoen, R. Hooft, T. Kuhn, R. Kok, J. Kok, S. J. Lusher, M. E. Martone, A. Mons, A. L. Packer, B. Persson, P. Rocca-Serra, M. Roos, R. van Schaik, S.-A. Sansone, E. Schultes, T. Sengstag, T. Slater, G. Strawn, M. A. Swertz, M. Thompson, J.

- van der Lei, E. van Mulligen, J. Velterop, A. Waagmeester, P. Wittenburg, K. Wolstencroft, J. Zhao, B. Mons, *Sci. Data* **2016**, *3*, 160018.
- [43] Chemotion ELN Documentation. <https://chemotion.net/chemotionsaurus/docs/eln/about> (accessed 03/25/2022).
- [44] F. Fink, S. Benjamaa, A. Hoffmann, S. Herres-Pawlis *Chemotion ELN Erklärvideos*. **2022**, <https://doi.org/10.5281/zenodo.6356844>.
- [45] P. M. Schäfer, M. Fuchs, A. Ohligschläger, R. Rittinghaus, P. McKeown, E. Akin, M. Schmidt, A. Hoffmann, M. A. Liauw, M. D. Jones, S. Herres-Pawlis, *ChemSusChem* **2017**, *10*, 3547–3556.
- [46] P. M. Schäfer, P. McKeown, M. Fuchs, R. D. Rittinghaus, A. Hermann, J. Henkel, S. Seidel, C. Roitzheim, A. N. Ksiazkiewicz, A. Hoffmann, A. Pich, M. D. Jones, S. Herres-Pawlis, *Dalton Trans.* **2019**, *48*, 6071–6082.
- [47] R. D. Rittinghaus, P. M. Schäfer, P. Albrecht, C. Conrads, A. Hoffmann, A. N. Ksiazkiewicz, O. Bienemann, A. Pich, S. Herres-Pawlis, *ChemSusChem* **2019**, *12*, 2161–2165.
- [48] R. D. Rittinghaus, J. Zenner, A. Pich, M. Kol, S. Herres-Pawlis, *Angew. Chem. Int. Ed.* **2022**, *61*, e202112853; *Angew. Chem.* **2022**, *134*, e202112853.
- [49] R. D. Rittinghaus, A. Karabulut, A. Hoffmann, S. Herres-Pawlis, *Angew. Chem. Int. Ed.* **2021**, *60*, 21795–21800; *Angew. Chem.* **2021**, *133*, 21965–21971.

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