

ELN Guide

Electronic laboratory notebooks in the context of research data management and good research practice – a guide for the life sciences



Imprint

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1. Introduction

1.1. What inspired this guide

More and more laboratories are replacing their paper lab notebooks with electronic laboratory notebooks, or ELNs.

But this transition is about more than just replacing paper with digital alternatives. It's also about finding ways to integrate electronic lab notebooks into an overarching digital research data management (RDM) system.

ELNs have a hugely important role to play in the documentation phase of the research data life cycle.

Anyone considering the option of purchasing and deploying an ELN should start by answering the following key questions:

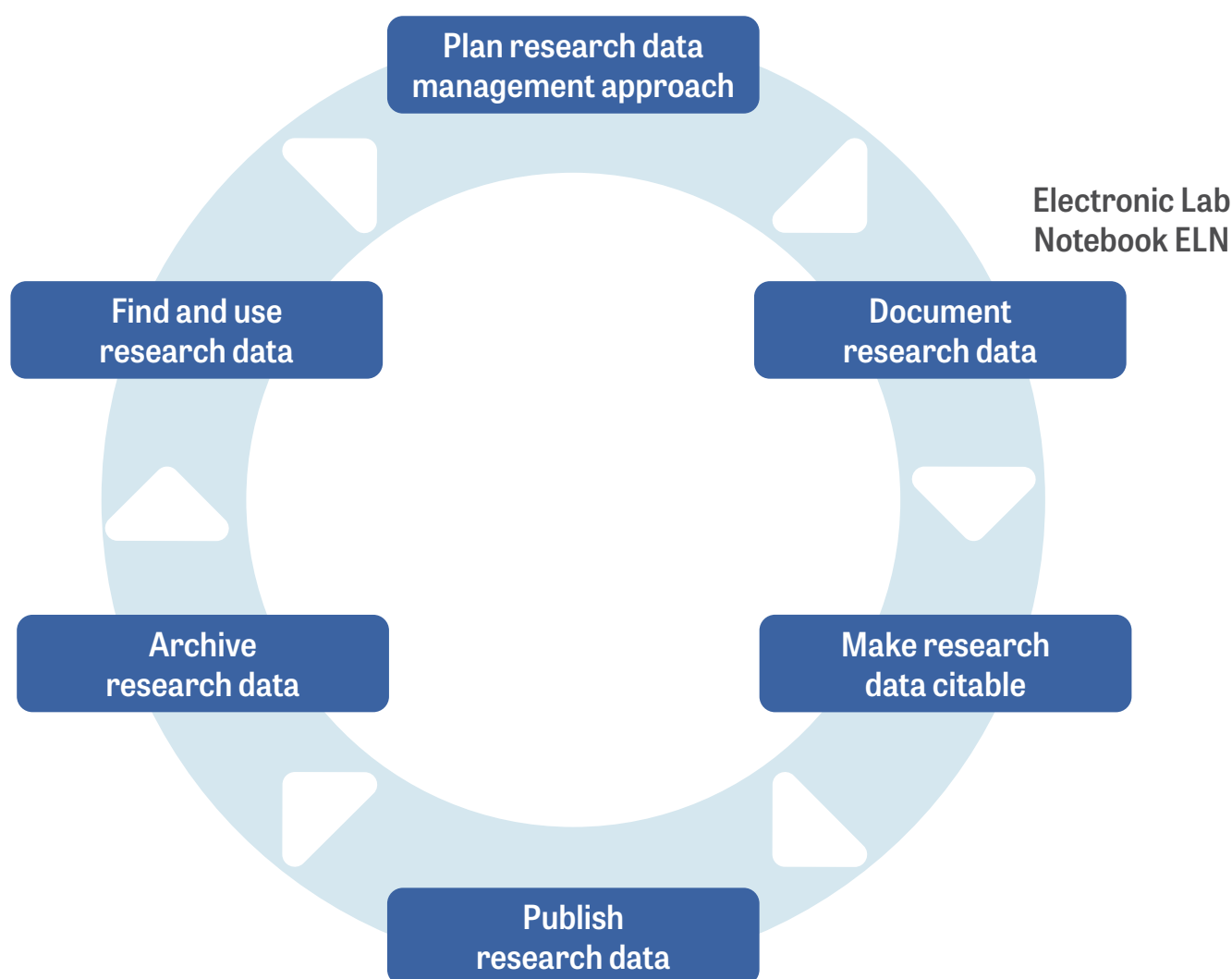
- ▶ What is the end-to-end workflow of research data over its entire life cycle?
- ▶ Which IT applications or tools should be used at each stage?

- ▶ What role should an ELN play in this overall context?

As well as helping to shape an institution's research data management strategy, an ELN can also make a major contribution to good scientific practice by making it easier to track and trace research processes and results over time.

Electronic lab notebooks offer a number of advantages in both these contexts, including:

- ▶ Direct integration/linking of data that is already available in a digital format (e.g. measurements, images, videos, audio files, text, tables)



Life cycle of research data

- ▶ Preventing loss of information due to illegible handwriting
- ▶ Search and filter functions
- ▶ Collaborative work functions (rights, role management)
- ▶ Ability to create and use templates (e.g. for repetitive processes)
- ▶ Embedded in a connected digital research environment (API, standard interfaces, import and export functions, links to repositories and other digital preservation systems etc.)

To find out more about switching from paper to electronic lab notebooks, the benefits of ELNs, and potential obstacles to introducing them, see the infobox on [Switching from paper lab notebooks to ELNs / Introducing ELNs.](#)



1.2. Purpose and objectives

The main purpose of this guide is to provide **practical advice** on introducing an electronic laboratory notebook, though it also includes a brief section explaining the science and theory behind ELN classification. Essentially, the task of introducing the right ELN to meet your goals can be divided into three phases, each with its own particular challenges. The first step is to select one or more products that might meet your needs. This is followed by a test phase, which ideally pinpoints one application as being the most suitable. Once the chosen ELN has been licensed and implemented, it is then distributed to the research groups.

One of the biggest hurdles in the selection process is the sheer variety of products available. There are almost one hundred in total, each with its own strengths, features and pricing structures. One of the primary goals of these guidelines is therefore to **help you define selection criteria** that reflect what your particular institution and laboratories actually need. This list of requirements can then be compared against the features offered by available electronic lab notebooks.

Legend



This symbol indicates an internal link. Clicking on the text after the arrow will take you to the relevant part of this document.

You can go back to your original place in the text at any time by pressing “Alt” + “Left arrow key”



Infoboxes contain links to further information (mostly hyperlinks to online resources). Information resources in the infoboxes are arranged by year of publication, with the most recent at the top.



Toolboxes contain tools that can be used as a template and adapted for your own use as required.



Best-practice-boxes feature a detailed description of a specific case study and can be read in parallel with the main text. The first best practice box, which appears immediately after this introduction, contains a summary of the interviews and includes links to jump straight to each individual case study.

It can be helpful to look at what others have done in this same situation, what their goals were, and what approach they took. That's why best practice examples form such an important part of this guide.

It also offers recommendations in the form of a checklist to help you take the most logical and systematic route to introducing an ELN.

1.3. How this guide is structured

Most of this guide focuses on recommended practical steps you can take to introduce an ELN into your institution. These steps aim to achieve the two key goals described above: integrating an electronic lab notebook into a broader research data management system, and improving research activities in line with good scientific practice.

The first part of the guide is about defining your requirements. This allows you to assess the different characteristics offered by available software tools and make the right choice for your needs.

At the end of this first section, we suggest some concrete steps that will help you select the right ELN systematically. To create this guide, we examined a series of ELN products that are relevant to the life sciences. As well as describing their core functions, we also identify key selection criteria. Our aim is to give you a preliminary idea of how well each tool meets the requirements of your specific institution or lab. Next, we offer recommendations on how to introduce an electronic lab notebook, including a sample needs assessment.

Lastly, we include some theory on how to draw up criteria for categorising ELNs.

As you progress through the guide, you will also come across a series of best practice examples. These are based on seven interviews we conducted with experts who already use an ELN tool, with all the interviews following the same basic pattern. Each example of best practice is divided into the same series of sections, including a background and needs analysis.

The final part of the guide is a checklist. This provides a general overview of the key things to bear in mind when introducing an electronic lab notebook. You can use the checklist to work through the individual steps one by one and jot down notes to sum up what you need from an ELN.



Switching from paper lab notebooks to ELNs / Introducing ELNs

Kanza S, Willoughby C, Gibbins N, et al.:
[Electronic lab notebooks: can they replace paper?](#)
J Cheminform. 2017;9(1):31. Published 2017 May 24,
DOI: 10.1186/s13321-017-0221-3

Office of Scholarly Communication:
[Paperless research' solutions – Electronic Lab Notebooks](#)
University of Cambridge, Unlocking Research, 2017

Ulrich Dirnagl, Ingo Przesdzing:
[A pocket guide to electronic laboratory notebooks in the academic life sciences](#)
Version 1, F1000Res. 2016, DOI:10.12688/f1000research.7628.1

Alan Wolf, Jan Cheetham:
[Electronic Laboratory Notebooks: More than Notes](#)
University of Wisconsin – Madison, 2015 (Video)

Pannabecker, Virginia:
[How Do Electronic Laboratory Notebooks Inspire Researchers?](#)
Poster presentation at MAC / MLA, Asheville, USA, 2015 (poster)

Colin L. Bird, Cerys Willoughby and Jeremy G. Frey:
[Laboratory notebooks in the digital era: the role of ELNs in record keeping for chemistry and other sciences](#)
Chem. Soc. Rev., 2013, 42, 8157-8175: First published on 17th July 2013, DOI: 10.1039/C3CS60122F

Jim Giles:
[Going paperless: The digital lab](#)
Nature, 2012

Klokrose, Clemens Nylandsted; Zander, Pär-Ola:
[Rethinking Laboratory Notebooks](#)
Proceedings of the 9th International Conference on Designing Cooperative Systems . ed. / Myriam Lewkowicz; Parina Hasanally; Markus Rohde; Volker Wulf. Springer, 2010. p. 119-139

Research data wiki
<https://www.forschungsdaten.org/index.php/Elektronische-Laborbücher>

Mailing lists:

- ▶ JiscMail RESEARCHNOTEBOOKS homepage (Email discussion lists for the UK Education and Research communities)
<https://www.jiscmail.ac.uk/cgi-bin/wa-jisc.exe?AO=RESEARCHNOTEBOOKS>
- ▶ GWDG data and IT service centre:
<https://listserv.gwdg.de/mailman/listinfo/elabnotebook>



BEST PRACTICE BOX

Best practice examples: survey methods and summary

1. Methods used

We conducted qualitative expert interviews to compile examples of best practice. The following criteria were used to select the case studies:

- ▶ Important to present open-source and in-house solutions as well as commercial products.
- ▶ Process of introducing the ELN should already have achieved a “visible level of maturity”.
- ▶ Interview people working in different roles in order to provide multiple perspectives on the topic

We collected the information for this guide in October and November 2018. THE interviews for the new case studies in this second edition were conducted in spring 2020. Nearly all the interviews were conducted by telephone and recorded; the only exception was University Hospital Cologne, which was close enough to allow the interview to be conducted in person and taken down in writing. The transcription was then used as the basis for creating uniformly structured texts.

The interview questions can be found in the → [Appendix](#).

2. Overview of case studies

Charité/Berlin Institute of Health (BIH):	ETH Zurich (Eidgenössische Technische Hochschule Zürich):	Leibniz Institute on Aging - Fritz Lipmann Institute (FLI)	Heinrich Heine University (HHU) Düsseldorf:	Robert Koch Institute (RKI) Berlin:	University of Göttingen (UMG):	Cologne University and University Hospital Cologne
Commercial product: Labfolder	Developed in-house and published under open source licence: openBIS	Commercial product: Rspace	Open source licence: eLabFTW Commercial product: Labfolder	Developed in-house: LIMS with ELN module	Commercial product: RSpace	Commercial product: eLabJournal
Link to Charité/BIH case study	Link to ETH case study	Link to FLI case study	Link to HHU case study	Link to RKI case study	Link to UMG case study	Link to UzK case study

3. Summary of interviews

1. Background

Research data management (RDM) and ELNs have been a key subject of debate at many institutions for a number of years. These discussions generally involve staff from multiple areas of the organisation. This has yielded different perspectives and approaches:

- ▶ Researchers and professors tend to take more pragmatic approaches that reflect their day-to-day realities. Only later does their focus switch to ELNs in the broader context of research data management and integration.
- ▶ Lab managers tend to initially focus on LIMS (Laboratory Information Management System) functionalities and on ensuring QM compliance and the use of standard operating procedures (SOPs) that can be clearly defined and documented.¹
- ▶ IT professionals tend to take a more systematic approach and to view the system in its overall context right from the start. They emphasise the importance of close cooperation with labs to gain the necessary understanding of their processes and requirements.

- ▶ Librarians are often entrusted with the task of developing accompanying information and training courses, offering advice, and supporting key processes (e.g. linking the ELN to a repository). However, libraries can also play a leading role in the introduction of electronic lab notebooks.

Typical situations prior to the introduction of an ELN:

Various labs at an institution, each of which is on a different stage:

- ▶ Some research groups are still using paper notebooks, mostly in a hybrid form, while others have already developed their own database systems or come up with DIY solutions using tools such as note-taking software.
- ▶ Individual laboratories are asking to introduce an ELN or drawing up requirements for a digital data management system.
- ▶ Research groups and their managers express an interest in improving scientific practice.
- ▶ A university is planning to provide technical and organisational solutions for its institutes.
- ▶ The topic is initiated and developed within the context of a funding programme.

2. Needs analysis

The needs of the laboratories and researchers are usually determined systematically using an Excel spreadsheet or similar tool. Time is often a limiting factor in obtaining this information, so alternative options may also be used, such as talking directly to the people involved to assess their needs or organising one-on-one or group discussions.

- ▶ A common outcome of the needs assessment is that none of the commercially available systems meet all the requirements.
- ▶ Other factors also play a role in addition to people's needs, for example price, usability, and in-house resources.
- ▶ Everyone who was interviewed had at least considered developing a solution in-house or using an open-source solution.

3. Decisive criteria for selecting a specific solution and key benefits

Reasons for choosing a commercial product:

- ▶ The product meets your needs.
- ▶ Option of cooperating with the vendor to allow your own change requests and additions to be incorporated into ongoing product development.
- ▶ The product meets the conditions set by a lab for purchasing a product because it has the functionalities they need (e.g. depiction of chemical structures).
- ▶ The vendor can provide training and support.

Reasons for choosing an open-source product or developing a solution in-house:

- ▶ You wish to add a free generic solution to complement a commercial tool that has already been introduced.
- ▶ Adapting a commercial product would be too time-consuming and expensive.
- ▶ Human resources are available in-house to develop a solution.
- ▶ Existing in-house solutions or preliminary work can be built on.
- ▶ Ability to implement a solution step-by-step based on evolving requirements without having to depend on a vendor.

4. Implementation

There may be obstacles to overcome outside the research departments, such as the staff council and/or statutes.

Successful implementation of a solution relies on support from users, especially in the initial phase, and measures for achieving acceptance.

Costs can be covered by funding programmes.

For in-house and open-source solutions:

- ▶ Iterative approach.
- ▶ Agile software development methods, i.e. a software development process that increases transparency and flexibility from the start. This should lead to faster system deployment, thereby minimising development risks.ⁱⁱ
- ▶ Step-by-step approach in close consultation with users.
- ▶ In-house development of training and information materials.

For commercial products:

- ▶ A certain amount of IT resources must be available for updates/troubleshooting/administration.
- ▶ Training is provided by the vendor.

5. Current status

All the ELNs highlighted in the interviews have either already been introduced and established or are currently being implemented. The interviews include information on how many users are already using the tool, which solutions the organisation is working on to integrate the ELNs into an RDM, and which stage the project has currently reached.

6. Lab system in the context of RDM

All the interviewees emphasised the importance of integrating the electronic lab notebook into an existing or future research data management system. This currently focuses on the following aspects:

- ▶ Raise awareness of the need for RDM, for example through training programmes.
- ▶ Connect the ELN to repositories and digital preservation systems.
- ▶ Create central storage locations/systems.

7. Summary

There is no “one-size-fits-all” answer to the question of whether to develop a solution in-house or opt for an open-source or commercial product. Each option offers its own opportunities and risks. To make an informed decision, it is important to carefully examine and analyse the needs and requirements in each case.

Good user support is an essential prerequisite for the successful introduction of an electronic lab notebook.

Developing standard formats for exporting data from electronic lab notebooks is an important step towards facilitating data exchange between systems.



BEST PRACTICE BOX

Case study: Charité Berlin/Berlin Institute of Health
commercial product: Labfolder

Expert interviewed: Professor Ulrich Dirnagl, director of the Department of Experimental Neurology at Charité – Universitätsmedizin Berlin (basic research department with around 100 employees divided into seven to eight independent workgroups) and founding director of the Quest Center at the Berlin Institute of Health.

1. Background

- ▶ The Department of Experimental Neurology employs all the techniques typically used in biomedical basic research, such as microscopy, molecular biology, cell culture, in vivo animal experiments, and imaging with magnetic resonance tomography. These activities produce large quantities of data.
- ▶ Professor Dirnagl has spent more than a decade investigating ways to improve research, focusing in particular on the use of lab notebooks within the context of research data management.
- ▶ He and his colleagues were aware that their existing set-up did not meet the latest standards of effective research and data security. They therefore decided to introduce an electronic lab notebook to replace paper lab notebooks as a documentation tool.

2. Needs analysis and decision-making process

- ▶ The team discussed and evaluated whether it made sense to develop a solution in-house. Their considerations were based on two key points: the immaturity of the electronic lab notebook market around 10 years ago, with relatively few products available, and the institute's philosophy of maximising its use of open-source software. The pros of in-house development included the programming skills and expertise of some of the institute's employees. The cons included the complexity of the task and the need for regular ongoing development work.
- ▶ The various products were tested for one or more weeks to obtain an overview and get some first impressions of each option. The idea of extending these tests to a real-life context for six-month periods and then potentially switching to the next candidate was discounted due to the unreasonable workload this would place on employees.

3. Decisive criteria for selecting a specific solution and key benefits

- ▶ The idea of developing a solution in-house was rejected due to the complexity of the task and the ongoing need for development and adaptation. Concerns were also raised about the legal requirements for ensuring evidentiary value. The team was aware of a case in

which the U.S. Food and Drug Administration (FDA) refused to accept data documented using an in-house solution.

- ▶ The decision to opt for the commercial product “Labfolder” was based on its positive test results and the following additional criteria:
 - The vendor's headquarters are close by in Berlin.
 - Labfolder's background lies in the same research discipline.
- ▶ Labfolder enables cooperative development by providing access to a test environment and designated contacts to help assess newly developed features. Labfolder is willing to incorporate changes requested by the user as long as they could be of broader interest

4. Implementation

- ▶ Training was carried out by the vendor.
- ▶ A team of employees skilled in IT supported the roll-out and operation of the solution:
 - Software set-up: creating and assigning roles
 - System administration.
 - Applying updates.
 - Troubleshooting in the event of a system crash.
 - Help with problems and questions.
- ▶ Measures for achieving acceptance:
 - Major emphasis was placed on onboarding as a means of ensuring the new solution was introduced successfully. This involved asking staff members who were already familiar with the electronic lab notebook to actively support new users in order to prevent them becoming frustrated and ceasing to use the ELN.
 - Use of the ELN forms part of the department's internal guidelines. Compliance with these guidelines is a determining factor in the distribution of resources and funding.
- ▶ Hurdles had to be overcome outside the research environment:

- Persuading the staff council that the ELN is not a tool for monitoring employees.
- Making the necessary changes to the charter to ensure that the ELN has equal status to that of paper lab notebooks in terms of good scientific practice for documenting research work.

5. Current status

- ▶ ELN still being used successfully both in the Experimental Neurology research department and in many Charité workgroups.
- ▶ The QUEST Center currently supports 1,000 people in using the system. The goal is to roll this out to the entire research community (max. 7,000 people).
- ▶ Administration and maintenance at the QUEST Center is handled by an IT specialist. This task is carried out at Charité by a team of employees skilled in IT.

6. Lab system in the context of RDM

- ▶ Use of the electronic lab notebook raises awareness of the importance of research data management.
- ▶ The plan is to set up a storage system for object-oriented storage and archiving in cooperation with the IT department. Key questions include:
 - How does the institute currently back up its data?
 - How can we guarantee the preservation of data for ten years?
 - How can the institute get access to data when employees leave?
- ▶ Labfolder stores data up to a certain size in the system database, i.e. ‘in the lab notebook’. Pointers are used to reference large files, which are stored on the Charité’s archive servers. A solution must be found to preserve long-term access to the linked data.
- ▶ Possible link to a repository in cooperation with the library:
 - Establishing a structure for the “Refubium” repository run by Freie Universität Berlin.
 - The plan is to find an automated way to make green open access publications available in the repository. This will then be extended to gold open access publications.
 - It is important that research data can be automatically transferred from the ELN to the repository via API.
 - Some psychological hurdles will need to be overcome: publication in the repository relies on users entering full and proper documentation in the ELN.

7. Summary

For most researchers, it is only when they start getting to grips with an electronic lab notebook that they understand what research data management involves and why it is so important. As a rule, researchers store their data on a virtual drive provided by the institute without knowing its actual location. In some cases, researchers also store data on their lab computer or portable hard drives. Professor Dirnagl argues that one of the biggest benefits of electronic lab notebooks for RDM is the fact that it raises awareness of this topic in the first place. At Charité, this extends into setting up a research data management system in collaboration with the IT department. The electronic lab notebook is the starting point for this process.

8. Find out more

- ▶ Links to QUEST/Freie Universität Berlin
 - <https://www.bihealth.org/en/research/quest-center/service/eln>
 - <https://www.bihealth.org/de/quest-center/mission-ansatze/open-science/quest-toolbox/>
 - <https://www.bihealth.org/en/notices/press-release-research-40-berlin-institute-of-health-moves-to-electronic-lab-notebooks>
 - <https://refubium.fu-berlin.de/?locale-attribute=en>
- ▶ Publications

Ulrich Dirnagl and Ingo Przesdzing: [A pocket guide to electronic laboratory notebooks in the academic life sciences](#), 2016. DOI: 10.12688/f1000research.7628.1
- ▶ Presentation

Prof. Dr. Ulrich Dirnagl: **Nie wieder ohne – das elektronische Laborbuch aus der Sicht eines Neurowissenschaftlers**, [Never going back – an ELN from a neuroscientist’s perspective], Helmholtz open science workshop on electronic lab notebooks, 2018-09-14
Download the slides: https://os.helmholtz.de/fileadmin/user_upload/os.helmholtz.de/Workshops/elN18hzi_dirnagl.pdf (PDF)

2. The electronic lab notebook in the context of research data management

2.1. Documenting research data in an ELN

A lab notebook serves to document the research process and the research data this produces. The ability to publish and reuse research data and ensure the verifiability of research results relies on complete and fully traceable documentation. However, good documentation is time-consuming, which means it is often neglected in the course of everyday lab work. That leads to research results that can be neither reproduced nor referenced, i.e. that are difficult to reuse. ⁱⁱⁱ

It is important to remember that over ninety percent of all data in the life sciences is now digital. As well as allowing researchers to document raw data without switching between different media formats, an ELN makes research results traceable and reusable. That's because it ideally allows lab protocols, processes and workflows to be directly linked to the raw data they yield.

What's more, it paves the way for significant time savings and knowledge transfer in day-to-day lab work by facilitating the creation and use of templates for protocols, processes, standard operating procedures (SOPs) and workflows. ELNs can become a valuable knowledge resource by describing data and combining this with a good search function; some ELNs also help create metadata.

2.2. ELNs as a key component of the research data life cycle

Increasingly, funders require researchers not only to submit a data management plan (DMP), but also to store research data in a way that makes the data reusable and the research process transparent and traceable. At the same time, more and more publishers are insisting that the research data on which a text publication is based should be archived and published.

An electronic lab notebook can be of great help in meeting these requirements, especially if it is integrated into an existing or planned research data infrastructure. This requires a high-quality, well documented application programming interface (API).


As the case studies show, the introduction of an ELN often provides the initial spark for thinking about research data management and starting to put together solutions. Ideally, this results in the creation of an integrated overall system in which the ELN can exchange data with the other components in the management process.

One of the key tasks is the on-demand provision of research data and results recorded in the ELN to repositories and digital preservation systems.

Another important factor is the integration of data provided by other research software, e.g. formula editors, statistical programmes, visualisation tools, analysis software, and devices such as microscopes.

Questions must also be answered on which strategies to use for centralised data storage and how to provide the necessary hardware to meet demand.

Check out suggested solutions

- ▶ in the examples of best practice in the section on “Lab systems in the context of research data management”.
- ▶ in the  [infobox “ELNs as a key component of the research data life cycle”](#).



BEST PRACTICE BOX

Case study: ETH Zurich
openBIS - in-house solution with open source licence

Expert interviewed: Dr Bernd Rinn, Head of Scientific IT Services (SIS) at ETH IT Services.

1. Background

- ▶ The national systems-biology funding initiative in 2007 initiated the development of a research data management system for collaborative research projects. Start of openBIS development, decision to make the platform open source.
- ▶ Since 2009, openBIS has been developed in its current form as a database platform. Continuous improvements have been made, driven by a constant awareness of researchers' needs and efforts to meet these with new features. Initially, development therefore focused on LIMS-style functionalities and on the characteristics of data produced in a laboratory and the ways in which this data is collected.
- ▶ Since 2012, there has been considerable interest in the idea of introducing a system combining ELNs and LIMS. Impetus for evaluating such a system came from several research groups in different departments of the life sciences.
- ▶ Founding of Scientific IT Services (SIS) in 2013, a unit that aims to support researchers with dedicated IT systems. SIS focuses on the operation and improvement of ETH's high-performance computers, data analytics clusters, scientific software development, and research data management.

2. Needs analysis and decision-making process (multi-step)

- ▶ Are suitable commercial solutions available? Price was the main criterion; paying the high six-figure cost of systems that were developed for the pharmaceutical industry was out of the question. Four offers met the pricing criteria.
- ▶ These four candidates were invited to tender. Two accepted, the other two were not interested.
- ▶ One of the laboratories requested that the evaluation should also include the product that was previously developed in-house at ETH in collaboration with another lab.
- ▶ Usability testing was conducted for a total of three products: the two commercial solutions and the product developed in-house.

★ BEST-PRACTICE-BOX

Case study: ETH Zurich
openBIS - in-house solution with open source licence

- ▶ Price comparison of the two commercial offerings in both their cloud and on-site versions.
- ▶ Technical evaluation criteria drawn up by SIS:
 - **programming interfaces:** ELN/LIMS is part of a system and must be integrable.
 - **bulk export capabilities:** it must be possible to export all the data together should it become necessary to migrate to a different system.
 - **risk assessment:** where do we think our risk lies if we opt for this solution?
- ▶ Presentation of the results in a matrix and joint review involving professors and lab managers.
- ▶ **Results:** None of the systems tested has the required functionalities and is sufficiently user-friendly.

3. Decisive criteria for selecting a specific solution and key benefits

- ▶ The product developed in-house has sufficient potential and can be expanded.
- ▶ Those involved are able and willing to work through a longer process of adaptation.
- ▶ Developing a common system will allow synergies to be harnessed.

4. Implementation

- ▶ In collaboration with other universities, submission of the “Data Life Cycle Management (DLCM)” project as part of the “Scientific Information” national research funding programme.
- ▶ DLCM ran for three years from around the end of 2014.
- ▶ Launch of the “Active data management” workstream in the DLCM project.
- ▶ Electronic lab notebooks are one aspect of active data management.
- ▶ Further development of use cases originally developed in ETH laboratories.
- ▶ Comparison with systems used/developed at other universities.
- ▶ Adjustment and expansion of in-house gap analysis designed to identify strategic and operational gaps.
- ▶ Inclusion of non-life science laboratories, e.g. Experimental Astrophysics in Geneva.

- ▶ Development of software to close the gaps identified in the previous step.
- ▶ Regular release of new versions:
 - to develop new functionalities,
 - to improve usability.
- ▶ Iterative approach.
- ▶ Updates developed in cooperation with the laboratories based on their needs (step-by-step approach).

5. Current status

- ▶ openBIS is a database platform developed at ETH Zurich. The platform has plug-in interfaces for programming modules. As well as developing your own plug-ins, it is also possible to use modules developed by others. Apart from ETH, a number of external groups have also developed plug-ins which they continue to maintain and improve.
- ▶ The experiment description lies at the heart of the ELN/ LIMS plug-in developed at ETH Zurich.
- ▶ Visualisations can be used to show connections. Everything is linked together, including:
 - materials and samples in their electronic form
 - protocols and SOPs
 - raw data
 - models and processed data
 - results suitable for publications
 - the source code used to compile the results and the analysis notebooks.
- ▶ Connections to workflows bring together the experimental and theoretical sides of research (“wet lab and dry lab”), taking account of the fact that data is also subject to constant analysis.
 - Jupyter integration: with authorisation in openBIS, a Jupyter Notebook can be launched and an analysis workflow can be carried out with the data from openBIS. The results can be written back into openBIS.
 - KNIME interface (Konstanz Information Miner platform developed at the University of Konstanz).
 - Integration snippets to various other tools and analysis workflows.

- ▶ Other functionalities include
 - manual upload options,
 - connections to measuring instruments, and
 - data import.
- ▶ openBIS is being rolled out as a basic service throughout ETH Zurich. Individual groups also run other solutions in parallel.
- ▶ Courses are offered in both the basic concepts of data management and the specific skills of using the tool.
- ▶ open RDM.swiss is a follow-up project to DLCM. It aims to extend the service to the national research community in Switzerland.

6. Lab system in the context of RDM

- ▶ Cooperation with the library within the framework of the DLCM project.
- ▶ Two systems were set up:
 - Long-term digital preservation – running since 2012, based on the Rosetta digital preservation system.
 - Research Collection - repository based on Dspace; together with Zenodo, this is currently the most used repository in Switzerland according to a survey by the Swiss National Science Foundation.
 - The plan is to connect openBIS to both systems; the connection to the repository is already in progress.
- ▶ An archiving module based on openBIS was developed to handle the technical IT side of archiving data. This involves storing large data sets in affordable tape drive archives in order to reduce the cost of storing research data that is not actively managed. Rosetta is used for the digital preservation of data on the software side.
- ▶ Raising awareness of data management is of paramount importance.

7. Summary

Looking back over the past few years, it is clear that there was really no alternative to developing a solution in-house on an open-source platform. There continue to be numerous change requests, many of which include very specific requirements. Tackling this situation with a commercial product seems almost impossible, since it would require enormous flexibility on the part of the vendor.

8. Find out more

- ▶ Further ETH/SIS links
 - <https://labnotebook.ch/>
 - <https://ethz.ch/services/en/service/a-to-z/research-data/active-data-management/resources-for-ardm.html>
 - <https://sis.id.ethz.ch/>
 - https://siscourses.ethz.ch/rdm_training/ARDM-workshop-20180614.pdf (PDF)
- ▶ Publications:
 - Caterina Barillari, Diana S. M. Ottoz, Juan Mariano Fuentes-Serna, Chandrasekhar Ramakrishnan, Bernd Rinn, Fabian Rudolf: [openBIS ELN-LIMS: an open-source database for academic laboratories](#) *Bioinformatics*. 2016 Volume 32, Issue 4, Page(s) 638–640. Published online 2015 Oct 27. doi:10.1093/bioinformatics/btv606
 - Angela Bauch, Izabela Adamczyk, Piotr Buczek, Franz-Josef Elmer, Kaloyan Enimanev, Pawel Glyzowski, Manuel Kohler, Tomasz Pylak, Andreas Quandt, Chandrasekhar Ramakrishnan, Christian Beisel, Lars Malmström, Ruedi Aebersold, Bernd Rinn: [openBIS: a flexible framework for managing and analyzing complex data in biology research](#) *BMC bioinformatics* 2011 Volume 12, Page(s) 468 Published online 2011 Dec 8. DOI: 10.1186/1471-2105-12-468
- ▶ Presentations:
 - Bernd Rinn: **Electronic Lab Notebooks, Processes, Tools and Experiences: an ETH Zurich Perspective**, workshop on ELNs at RWTH Aachen University, 20.11.2017
Download the slides <https://rwth-aachen.sciebo.de/index.php/s/5OCOay7ocj4w9be#pdfviewer>
 - Caterina Barillari: **openBIS – an open resource for academic laboratories**, Helmholtz Open Science Workshop on electronic lab notebooks, 13.9.2018
Download the slides https://os.helmholtz.de/file-admin/user_upload/os.helmholtz.de/Workshops/elni8hzi_barillari.pdf (PDF)

3. What features should an electronic lab notebook have?

In addition to laboratory-specific needs, there are also some basic requirements that all electronic lab notebooks should meet. Some of these are of a general nature, while others apply to specific activities or actions, though the boundaries are not always clear.

For example, having suitable exit strategies is a key consideration for researchers who want to take their data and results with them if they move to a different institute. But this issue may also be important on an institutional level, for example if the need arises to switch to a different product.

For a more detailed discussion of exit strategies, see section 3.10. → [Exit strategies](#).

3.1. Ability to replicate research processes

The electronic lab notebook must be capable of replicating and depicting the entire research process, including use cases, methods and the details of each experiment (i.e. data, observations, materials, protocols and procedures, reactions and calculations, results and conclusions).

3.2. Ability to capture unstructured data

Many researchers emphasise the importance of being able to capture and store data in the kind of unstructured way that is possible in a paper lab notebook. Electronic lab notebooks should enable this option, for example by allowing researchers to enter text and make sketches. This option is often referred to as “just a white sheet of paper”. Other types of unstructured data include video and audio files. The ability to annotate unstructured data with meaningful metadata guarantees their findability and thus their reusability. This is a significant advantage of ELNs compared to paper lab notebooks.

3.3. Usability

Usability is an important criterion, because experience suggests that once users have abandoned a software product, it is difficult to win them back.^{iv} Clarity is therefore preferable to feature overload. Key characteristics of a user-friendly interface include intuitive operation, easily-navigable menus and drag & drop. Research groups are often international, so a tool’s multilingual capabilities may also be a significant factor.

For more links to usability resources, see the [infobox “What should an ELN offer?”](#)

3.4. Transparency and flexibility

ELNs should be capable of displaying projects and experiments clearly and vividly and offer flexible ways to arrange and configure them. If necessary, it should be possible to display workflows in both a project-specific and cross-project context. It therefore makes sense to analyse the workflows in advance to determine which ones the ELN will need to depict. If the ELN will be used by research groups with different requirements – for example, groups from different domains – then it must be adaptable enough to adapt to their different needs.

To find out more about analysing workflows, see the [infobox “What should an ELN offer?”](#)

3.5. Performance and stability

It is important to choose an ELN vendor that has a stable and solid business so that the product will continue to be improved and adapted to new technologies. Some vendors already have an established market presence and may even offer various other types of products in addition to ELNs. For less-established companies, the following questions can help to assess a company’s stability:

- ▶ How long has the company been in business?
- ▶ Does it have enough capital investment to get through crises?
- ▶ Can it provide references?
- ▶ How many people does the company employ? Does it have a professional development team?
- ▶ Do its employees have a research background and/or many years of laboratory experience?

Equally important are the stability and reliable performance of the software itself, since these are critical to ensuring data is documented smoothly and efficiently. Instead of relying on test data and small test files, run more extensive tests that are as close to reality as possible. It is also advisable to run performance tests to check the software’s responsiveness and stability when handling larger data sets.

For more links to stability resources, see the [infobox “What should an ELN offer?”](#)

3.6. Compliance with regulatory requirements

If the laboratory or research group is subject to regulatory requirements, make sure to choose an ELN that will ensure compliance.

Examples of regulatory requirements:

GxP:

“GxP” is an abbreviation for generic good practice. The G stands for good, the P for practice, and the x for the various fields of application.

Examples include GLP (good laboratory practice, see below), GRP (good research practice) and GMP (good manufacturing practice).

GLP:

A quality system concerned with the organisational process and the conditions under which non-clinical health and environmental safety studies are planned, performed, monitored, recorded, archived and reported.^v

ISO – International Organization for Standardization:

A global network of national standards bodies which develops and publishes standards.^{vi} Thus, an ISO standard is a standard set by the ISO.^{vii}

HIPAA:

U.S. Health Insurance Portability and Accountability Act: rules that protect the privacy of patients and ensure the security of healthcare data.

To find out more about regulatory requirements, see the  [Infobox “What should an ELN offer?”](#).



ELNs as a key component of the research data life cycle

Samantha Kanza, Nicholas Gibbins & Jeremy G. Frey:

[Too many tags spoil the metadata: investigating the knowledge management of scientific research with semantic web technologies](#)

Cheminform 11, 23 (2019), DOI: 10.1186/s13321-019-0345-8

Jan Potthoff, Patrick Hodapp, Bernhard Neumair, Stefan Bräse, Nicole Jung:

[Procedures for systematic capture and management of analytical data in academia](#)

Analytica Chimica Acta: X, Volume 1, March 2019, DOI: 10.1016/j.acax.2019.100007

Nicole Jung:

[Chemotion ELN – basic functions and special applications](#)

Helmholtz open science workshop on “Electronic lab notebooks” 2018

Machina, Hari K.; Wild, David J.:

[Electronic laboratory notebooks progress and challenges in implementation](#)

Journal of laboratory automation, Volume 18, 2013, Issue 4, pp. 264-268





BEST PRACTICE BOX

Case study: Leibniz Institute on Aging, Jena
(Fritz Lipmann Institute, FLI), commercial product: RSpace

Experts interviewed: Dr Karol Szafranski, Georg Peiter. The Core Facility (CF) Life Science Computing, which is run by Dr Szafranski, was tasked with introducing the ELN. It began the process in mid-2018 and continues to provide support and monitoring. As an FLI scientific technology and service facility, the CF also acts as a link between the research groups and an IT infrastructure. It channels the needs communicated by researchers and scientists into the development of IT and technical solutions. In early 2017, Georg Peiter was given the task of conducting market research, finding and evaluating products, and preparing the invitation to tender.

1. Background

- ▶ The initial steps to procure an electronic lab notebook were taken in 2016. A list of criteria was compiled based on the relevant literature. This was voted on by FLI group leaders and, starting in early 2017, gradually developed into a practical and comprehensive list of criteria. Following a case of research misconduct, the FLI updated its strategy to incorporate the rules of good research practice (GRP). One of the core elements of its comprehensive list of GRP measures was the institute-wide use of an electronic lab notebook. This measure was to be implemented before a special evaluation scheduled for September 2019. The use of the ELN was made obligatory in order to facilitate the comprehensive, centralised documentation of research data. Criteria development, procurement, installation and commissioning were carried out from 2017 onwards by the Head of Core Facilities, Dr. Matthias Görlach, and the scientific supervisor of the Core Facility Life Science Computing, Prof. Steve Hoffmann.
- The unacceptable effort required to adapt heavily structured solutions due to the very heterogeneous range of methods used throughout the institute: the FLI conducts all kinds of molecular biology research, from simple biological lab techniques such as PCR, DNA analyses and Western blot right through to sequencing, protein mass spectrometry and high-resolution microscopy. In organisational terms, the FLI is currently divided into twelve experimental research groups, seven Core Facilities and two Animal Facilities. It was already using heavily structured electronic documentation systems as targeted solutions in a few limited contexts, e.g. in Animal Facilities. Structured systems were also regarded as an option for work groups with stable work processes, e.g. selected Core Facilities.
- Targets for the budget and timeline for the overall process. It became clear that complex ELNs would take too long to implement, so the system would not be properly established by the time of the special evaluation in autumn 2019.

2. Needs analysis and decision-making process

- ▶ Eliminated the option of open source solutions:
 - Examination of open-source projects published to date showed that none had a sufficient level of maturity to serve as a generic, institute-wide tool.
 - Another reason for ruling out open-source products was the lack of support from a manufacturer or third-party vendor. The FLI did not want to add the staff required to develop an open-source solution in-house and ensure viable ongoing operation.
- ▶ Drew up criteria to limit the range of products
- ▶ The FLI focused on a generic ELN (“blank piece of paper”), thereby excluding ELNs that store documentation in a heavily structured format. The reasons for this were
 - ▶ Eliminated the option of simple note-taking tools (e.g. OneNote, EverNote) which are not geared towards scientific use.
 - ▶ **Additional criteria determined to be necessary:**
 - On-premise data storage at the institute to guarantee data protection.
 - Purely browser-based solution that requires only an html5-capable browser to access.
 - Support for Good Scientific Practice:
 - Ability to comply with FDA 21 CFR Part 11 (criteria under which electronic records are considered trustworthy and reliable)
 - Ability to assign identity-based and role-based access rights

- Version history: every change must be traceable, every version must remain permanently accessible, mechanisms to ensure nothing can be deleted
- Ability to add a signature
- Internal links within the ELN/referenceability/ addition of clickable links, especially for large datasets
- Ability to assign tags to support search functions for documents
- Ability to collaborate by sharing lab notebooks and entries

▶ **Further criteria were defined, including:**

- **Comprehensive export capabilities:** ability to export in a range of human- and machine-readable formats that are also suitable for digital preservation systems, plus ability to export the entire ELN
- **Excellent usability:** a user-friendly interface is regarded as a key criterion for successfully introducing an ELN, since it is directly related to user acceptance of the tool
- Ability to link to files in the institute's data repositories
- Ability to export data, including to publicly accessible data repositories
- Ability to partially structure scientific documentation, e.g. using forms; using input masks with default values to facilitate input of metadata.
- Ability to search by title, full text content, tags

▶ **Steps to finalise the tender criteria:**

- Based on the criteria and specifications outlined above, some products were excluded in advance.
- To ascertain which criteria and functions were both necessary and desirable, the Core Facility took a closer look at two dozen ELNs.
- This process yielded three ELN solutions that were broadly representative of the available options. These were tested by a larger test group of researchers over a period of approximately six weeks. The testers met
- with the IT coordinators on a weekly basis to provide feedback which proved to be very helpful in drawing up the tender criteria.

▶ **Key factors for compiling the list of criteria:**

- Get future users involved at all stages of the product evaluation (from technical staff to group leaders).
- Teamwork and good communication between the Core Facility Life Science Computing (coordination), product testers from the group of future users, and guiding figures with authority to set standards, e.g. data protection officers, ombudsperson.
- Willingness of researchers to operate an ELN alongside their paper lab notebook and transfer documents from the paper notebook to the ELN on a trial basis.

3. Key benefits of purchased solution

- ▶ The vendor met all the tender criteria and submitted the most favourable bid within the tender framework.
- ▶ As well as providing the required export functions, the agreement signed with the vendor also offers protection against the vendor lock-in effect: use of the supplied software under a perpetual licence, long-term software support (10 years) and costs defined accordingly.
- ▶ User-friendly, intuitive user interface.
- ▶ A set of training resources provided by RSpace to meet ongoing needs, e.g. videos about standard processes
- ▶ **Further key benefits for the institute stemming from use of the ELN:**
 - Opportunities for cooperation: shared ELNs promote interaction within and between groups, helping people to work and collaborate more efficiently.
 - Digital data can be imported directly into the ELN as it emerges; scanned images can be annotated during import. Large quantities of data and data packages can be linked.
 - Templates can be created and reused as required. Scientists can also reuse their own written formulations to reduce time spent typing notes.

★ BEST PRACTICE BOX

Case study: Leibniz Institute on Aging Jena, (Fritz Lipmann Institute, FLI), commercial product: RSpace

4. Implementation

- ▶ Agreement on the mandatory introduction of an ELN had to be sought from the works council since the personal data stored in ELNs (e.g. time stamps, documentation densities) significantly affects employees' information rights. The data protection officer was already involved prior to the invitation to tender and was able to put forward his views back in October 2017 on the General Data Protection Regulation and compliance with EU data protection legislation. Once the product tender was completed, an agreement between staff and management was drawn up and signed within just ten months thanks to collaboration between the data protection officer, IT staff and the works council. This prevents the employer from using the ELN to collect data on how employees document their work or to use ELNs for closely monitoring employees. The works council also demanded a commitment from the institute to put all the necessary technical conditions in place to enable the ELN to be used. This covers employees' right to training as well as the availability of suitable terminal devices (for example procurement of additional tablets in cases where their use would be justified for lab work and lab documentation). In parallel with this company agreement, the Executive Board instructed that, following its introduction, use of the ELN for documentation would be mandatory as of 1 July 2019.
- ▶ During the introduction process, training of a total of 200 employees was staggered to ensure that key disseminators, or "multipliers" (i.e. those with a key role in lab work and group leaders) were trained first. This provided each working group with a dedicated contact for basic ELN questions. In this first phase, the main goal was to provide an overview of the system. Group leaders were empowered to make decisions, e.g. about the structure of data in their group or organising cooperation between staff members (e.g. by sharing documents). The next phase added broader training sessions that were opened up to all users on a voluntary basis. These face-to-face training sessions involved presenting the material to groups of up to twenty people. They continue to be offered at regular intervals. Currently, each session is attended by about five people. A key aspect of the training is to

reach mutual agreement at a group level on the way documents are organised, the key structuring tools in the ELN, and the use of standardised names when assigning tags. The introduction of the ELN has led to an increase in collaboration in some groups. The plan is to support this process by providing further training on organising collaborative work.

5. Current status and development

- ▶ **Monitoring:** Visits are currently being made to the individual research groups to get detailed feedback on the use of the lab notebook. The key focus here is on interaction between research staff and the IT experts responsible for the ELN. The question is how use of the ELN is organised in the lab and how real-life documentation works on a day-to-day basis. The goal is to identify where support is needed and how the processes could potentially be improved. One example was the finding that scientists are reluctant to use tablets for documentation, even though the physical distance between their lab workplace and their desk makes it impossible to enter documentation directly into a PC. Closer examination revealed that the existing tablets are unsuitable, which means it is currently easier to make a note on paper and transfer it to the ELN soon after. Improvements should be made here, e.g. by purchasing more suitable tablets, which should also be splash-proof and allow use with gloves.
- ▶ Satisfaction with the support provided by RSpace is high. As well as regular updates, the vendor also offers the option of getting involved in the design of future improvements. In addition, cost-based orders can be placed for features that are typically of interest to the institute. The vendor's openness to standardisation and format transparency is seen as positive.
- ▶ Additional specialist documentation capabilities might be introduced in the future for work groups in which highly routine procedures and standardised workflows are the norm. Specialised ELNs or other documentation systems would be a logical choice to partner with these new capabilities.

6. The laboratory system in the context of research data management

- ▶ The field of institutional data management is closely related to the topic of ELNs. It became clear in this case that choosing a generic tool means that systematic access to data and documentation will not be achieved until a later point in time. Creating archives of the data and written documentation is a separate challenge.

- ▶ Files can be exported from the ELN in pdf and xml formats, which are suitable for digital preservation systems.
- ▶ Primary data management was stipulated as one of the principles of GRP and is now being developed by a task force. Preparation of an invitation to tender for a new technical archiving solution is already underway.
- ▶ A future primary data store will also create a solution for persistent linking of files from the ELN.
- ▶ The connectivity and extensive export capabilities of the ELN were important selection criteria that are also key to the future implementation of a research data management system.
- ▶ The ELN itself is also suitable for archiving data in Dataverse. This could be a starting point for the development of a research repository.

7. Summary

- ▶ The key to identifying which criteria are necessary and desirable is to test the tools in an everyday work environment. This is especially true for checking whether the interface is user-friendly. It is vital to gain your own insights. Our experience suggests that videos, demos and tutorials from vendors are not sufficient. Almost all vendors will provide a test version on request. This allows researchers to test the product in everyday use and identify any hindrances to efficient documentation.
- ▶ The entire process of introducing an ELN and monitoring it during use must be constantly adapted to new developments. Choosing the next step to take often depends on feedback from users. For example, before the mandatory introduction of the ELN, we surveyed the level of user acceptance using a questionnaire. This revealed there were only a few research groups that still saw the ELN as disadvantageous compared to traditional lab notebooks. Extra support was therefore targeted at these research groups in the next stage.
- ▶ It is vital to keep in close touch with the intended users throughout the process, from product evaluation to introduction of the chosen solution.
- ▶ For example, resistance to the purchased product may subsequently emerge because some individuals feel they would have preferred a different product after testing. This is difficult to counter, but it underlines how important it is to keep communication channels open, seek opinions and involve users in the decision-making process in order to achieve the greatest possible consensus. Since labour law and data protection are both highly relevant issues, it is important to involve data protection officers and the works council in the process from a very early stage.
- ▶ The introduction of an electronic lab notebook is a highly complex process involving many users and groups. Systematic project management is therefore advisable. Not all of the details of this process can be predicted and controlled from the outset. That's why it's so important to maintain clear and comprehensive communication channels to ensure unforeseen obstacles can be eliminated with the involvement of future users and the institute's decision-makers. This prevents long delays and keeps the process moving forward productively.

8. Find out more

Related links:

- ▶ Link to the Core Facility Life Science Computing: <https://www.leibniz-flj.de/research/core-facilities-services/cf-life-science-computing>
- ▶ Website of the Leibniz Institute on Aging, Fritz Lipmann Institute: <https://www.leibniz-flj.de/>

Publications:

- ▶ **Karol Szafranski:** Inbetriebnahme der ELN-Software RSpace https://escience.aip.de/ak-forschungsdaten/wp-content/uploads/2018/11/FLI_RSpace_ELN.pdf
- ▶ **Georg Peiter:** ELN@FLI: Stage 0 - From market survey to performance specification https://escience.aip.de/ak-forschungsdaten/wp-content/uploads/2018/06/ELN_Peiter-FLI.pdf
- ▶ Digital und vernetzt – Elektronisches Laborbuch am FLI <https://www.beutenberg.de/aktuelles/nachrichten/news-details/digital-und-vernetzt-elektronisches-laborbuch-am-flj/>

3.7. Ensuring evidentiary value

Following the rules of good research practice requires research data not only to be fully documented, but also securely stored over the long term. ^{viii}

It is also in researchers' interests to ensure the results of their work are stored in digital form so that they have at least as much evidentiary value as a paper journal. The University of Kassel points out that a lab notebook is usually a private document. Provided with a signature, it offers evidence that the signatory has carried out certain experiments and obtained results. Compared to a conventional paper-based lab notebook, an ELN must fulfil specific legal requirements to have evidentiary value. One example is a certified electronic signature, which gives the document the same legal validity and effect as if it were signed by hand. ^{ix}

Definitions of key terms relating to evidentiary value:


FDA CFR 21 part 11: criteria established by the U.S. Food and Drug Administration (FDA) to govern the substitution of paper documents with electronic documents. ^x

Version management/versioning: traceable logging of all changes (i.e. with time stamp and user ID). Previous versions are saved and can be accessed again at any time.

Audit Trail: computer-generated, secure, time-stamped electronic records that make it possible to track the history of creation, modification and deletion.

Electronic signature and time stamp: data linked to electronic information that allows the signatory or signature creator to be identified and the integrity of the signed electronic information to be verified.

A time stamp demonstrates the legally valid time of the signature or change, regardless of the date and time of the local computer.

Check out a real-life example of the evidentiary value of electronic lab notebooks in the "Evidentiary value" section of the  [infobox "What should an ELN offer?"](#).

3.8. Deployment model/data storage

The methods chosen for deployment and data storage are significant factors in the ELN decision-making process. In some cases, an institute's data protection guidelines will force certain products to be excluded. For example, products that can only be operated as Software as a Service (SaaS) or using cloud storage may not be acceptable.

By storing the accumulated data on its own server, an institution retains full control over data and security protocols. This gives it responsibility for the security of the stored data and for ensuring its availability.

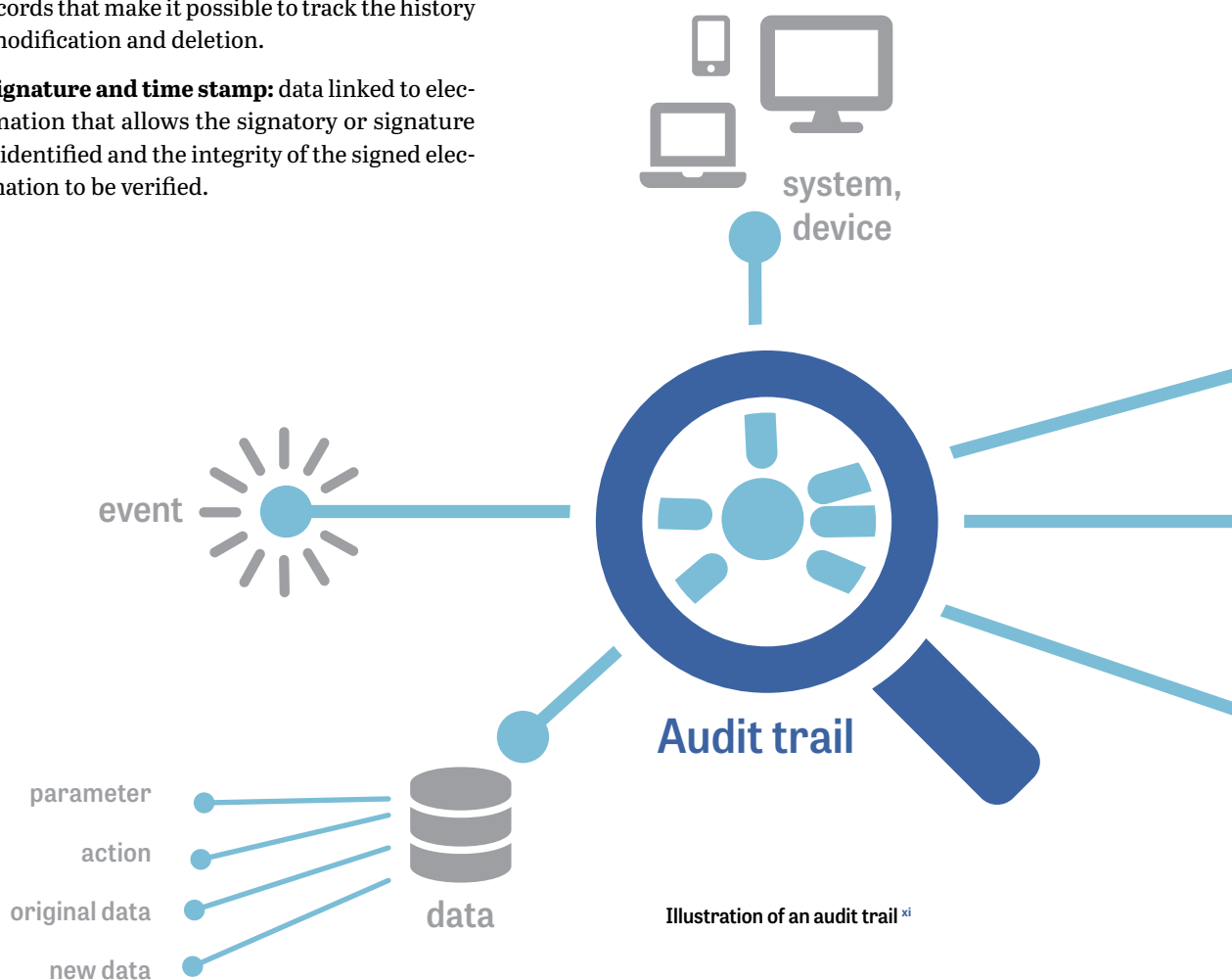


Illustration of an audit trail ^{xi}

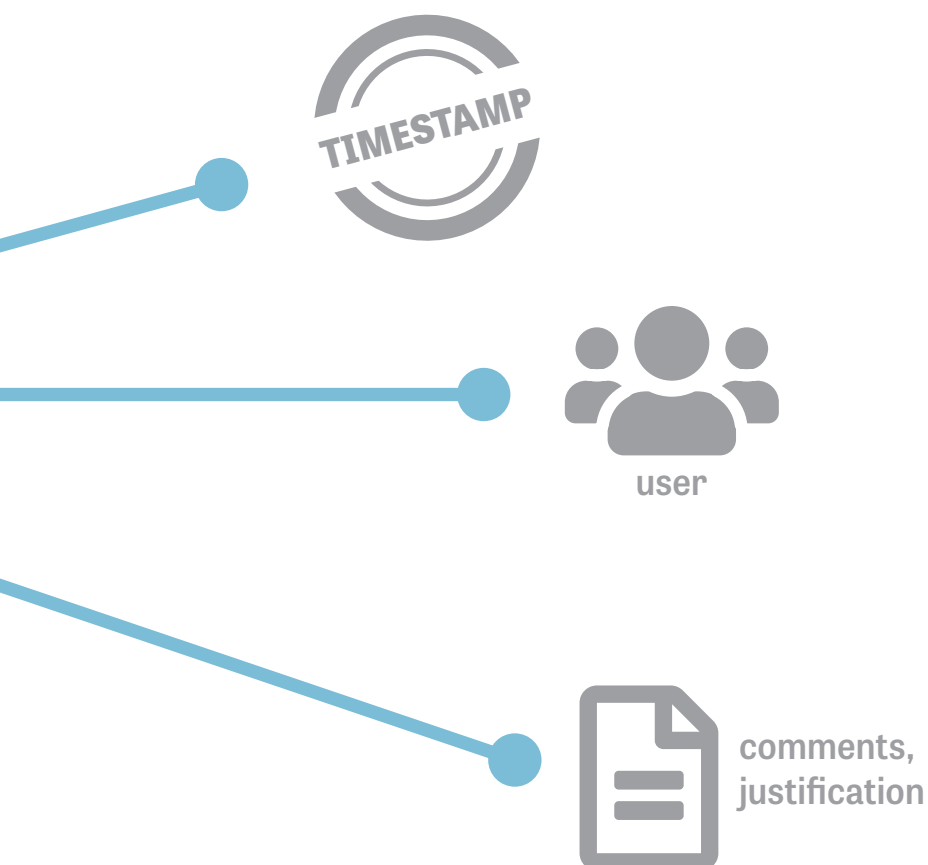
Choosing a solution that stores the data in the vendor's cloud shifts control of the data and data security to the solution provider. In this case, it is important to check where and how securely the data is stored. For example, a cloud hosted in Europe would generally be expected to have a higher chance of complying with European data protection regulations than a service based in the U.S. Some vendors take this into account by operating cloud servers located in Europe to store European users' data. This issue takes on particular significance when it comes to protecting personal and patient data, as stricter data protection regulations apply in Europe and Germany.

The main advantage of a pure cloud solution – where the vendor's cloud is used to run the software and store the data – is the ability to use the software without needing a separate IT infrastructure. This also eliminates the need for IT staff to take care of administration, maintenance, trouble-shooting, backup management, etc.

Cloud or on-prem deployment model?

SaaS (Software as a Service): The software and IT infrastructure are leased from a service provider for a subscription fee. Access is via an internet connection using a web browser. The data is stored in a cloud.^{xii}

On-prem: The software is provided for installation and use on the premises. Data can be stored on-site or in a cloud, which may be the user's own cloud.



3.9. Integrating ELNs into a research data management system or existing research data infrastructure

The following criteria should be considered when integrating devices into a research data management system:

Standard interfaces:

Seamless integration of frequently used programmes (e.g. ChemDoodle, GraphPad PRISM, FlowJo) without requiring programming skills.

API (application programming interface):

Programming interface that enables in-house applications (e.g. digital preservation system, repository) and/or devices and tools to be connected to an ELN. A comprehensive, well-documented API is the best option.

External linking:

Links to elements outside the system, e.g. large data sets that cannot be imported.


Internal linking:

Links to elements within the system, e.g. imported files.

Assigning metadata:

Digital documentation paves the way for making research data and results reusable as a valuable, searchable knowledge resource. This requires the content to be adequately described. Some ELNs provide support for adding metadata, for example in the form of input prompts and masks or automated “metadata harvesting” (e.g. filtering metadata from texts, exporting it from tables, extracting it from log files). It is important to note that the use of proprietary tools – i.e. software that restricts reuse, modification and adaptation rights and functions, ^{xiii} – can create obstacles to standardising metadata.


Check out a real-life example in the

 [infobox “What should an ELN offer?”](#).

Ability to assign persistent identifiers (e.g. ORCID, DOI):

Assigning persistent identifiers (PIDs) significantly improves the findability and citability of research data. A DOI (digital object identifier) provides a permanent link to a digital object, e.g. a text. An ORCID (Open Researcher and Contributor ID) is a PID for a specific person/institution.

To find out more about PIDs, see the

 [infobox “What should an ELN offer?”](#).

Seamless link to file sharing services and repositories:

File-sharing services (e.g. Figshare) and repositories (e.g. based on Dataverse software) are used by many researchers to share and publish research data. A seamless link can be created between the electronic lab notebook and these platforms, though this task must be tackled in cooperation with the vendor in the case of commercial products. Some ELNs come with these links already in place, in many cases based on previous customer requests.

3.10 Exit strategies: exporting the entire ELN

The decision to export an entire ELN may be based on economic or technical reasons. Commercial ELNs, in particular, store data in proprietary formats, which means that the data cannot be read or processed by other software products.

One reason for exporting an ELN from an economic standpoint is the vendor lock-in effect: if an ELN user is dependent on the vendor due to the proprietary nature of the software, this can have a financial downside if the vendor chooses to exploit this fact to dictate unreasonable price increases. It is therefore important to negotiate prices for the longest possible period when concluding a contract. Technical reasons for a complete export might include migrating to another system or setting up your own regular backups.

A suitable exit strategy allows the data – including all related information and structures such as links and files – to be exported in both a human-readable and a machine-readable format, for example as a database format.

Ideally, the exported data should be made available in a way that allows it to be migrated to another system without any loss of information. ELN software vendors are increasingly prepared to offer concepts that meet these goals.

3.11 Search function

One of the biggest advantages of electronic lab notebooks is the ability to find important data quickly and easily. In addition to full-text search, most products offer advanced search functions. There might include searching for chemical formulas, biological contents or tags, as well as features such as database queries and filtering options with flagging of filtered data records.

3.12 Functions for sharing / collaboration

The ability to share files, results and/or data is a key strength of electronic lab notebooks. While some products are tailored to individual users and groups, others can also be used throughout a department/institute or even across various institutions thanks to the option of creating multiple research groups.

Rights management settings can be used to make files read-only or grant read and write access, thus determining who can access each user's data and who is permitted to modify it.

Role management enables the creation of user roles (e.g. administrator, super user, user) with specific rights granted to each role. These roles can then be assigned to individuals. This avoids the need to assign specific rights for each individual user. For example, all group leaders could be assigned the role of super user with the rights to "create new group members" and "create new templates" plus "all the rights of the user role".



What should an ELN offer?

Workflows:

Vasa Curcin, Moustafa Ghanem, Yike Guo:

[The design and implementation of a workflow analysis tool](#)
The Royal Society, 2010, DOI: 10.1098/rsta.2010.0157

Stability:

[LIMSwiki.org page with an overview of ELN vendors:](#)

[LIMSwiki.org page with an overview of ELN vendors:](#)

Regulatory requirements:

Examples of GxP guidelines from Wikipedia:

https://en.wikipedia.org/wiki/Good_laboratory_practice

https://en.wikipedia.org/wiki/Good_documentation_practice

German Federal Institute for Risk Assessment (BfR) page on good laboratory practice:

https://www.bfr.bund.de/en/glp_federal_bureau-1488.html

European Commission guidelines on good manufacturing practice:

https://ec.europa.eu/health/documents/eudralex/vol-4_en

ISO: International Organization for Standardization

<https://www.iso.org/home.html>

Ensuring evidentiary value:

BeLab: Beweissicheres elektronisches Laborbuch, [Probative electronic lab notebook], a Kassel University project:

<https://www.belab-forschung.de/en/projekt.html>

Metadata:

Julia Menzel, Philipp Weil, Sara Y. Nussbeck:

[Metadata capture in an electronic notebook: How to make it as simple as possible?](#)

GMS Medical Informatics, Biometry and Epidemiology (MIBE), 2015 (PDF), DOI: 10.3205/mibe000162

Persistent identifiers (PID): DOI service:

DOI-Service:

<https://www.publisso.de/en/working-for-you/doi-service/>



BEST PRACTICE BOX

Case study: Heinrich Heine University Düsseldorf (HHU)
Open-source product (eLabFTW) and commercial product (Labfolder)

Experts interviewed: Maurice Schleußinger, Centre for Information and Media Technology (ZIM) at Heinrich Heine University, Research Data Management; Philipp Rehs, Central IT / High Performance Computing at ZIM

1. Background

- ▶ The Centre for Information and Media Technology (ZIM) engages with the topic of electronic lab notebooks to help meet the needs of the HHU institutes and support technical and organisational solutions.
- ▶ The commercial product Labfolder was introduced about five years ago.
- ▶ eLabFTW is currently being tested and is intended to add a generic and free alternative to the HHU's resources.

2. Needs analysis and decision-making process

- ▶ No needs analysis was performed because the time required to carry out and evaluate a survey is usually excessive and is seen as problematic. By the time the results are finally available and the chosen product is purchased, so much time has passed that some of the institutes involved may have already acquired their own solutions. This is undesirable since it leads to isolated 'silo solutions' that are neither connected to each other nor linked to the central research data management system. Once silo solutions are in place, it is difficult or impossible to persuade researchers to switch to a different product.
- ▶ Alternative approaches taken instead of a needs assessment:
 - Institutes that approach ZIM with certain requirements are introduced to the field of ELN services if it becomes clear during the consultation that electronic lab notebooks might be relevant to their needs.
 - The ZIM actively approaches institutes where they believe the topic could be relevant.

3. Decisive criteria for selecting a specific solution and key benefits

- ▶ Labfolder was introduced based on a specific request from an institute in the field of chemistry. It was regarded as the most suitable product for that particular laboratory/department at the time.
- ▶ In addition, an open-source product was introduced because
 - the costs of a Labfolder licence have to be passed on to the institutes and these costs represent an additional hurdle to adopting an ELN,
 - the ZIM wished to offer a generic, low-threshold tool that can be independently built upon by researchers with programming skills and integrated into their research environment.
- ▶ The decision to choose eLabFTW as a free alternative was made following an examination of various open-source products by the computer centre. Key criteria in favour of eLabFTW:
 - Specific enquiries had been made about this product by institutes.
 - The resources and skills were in place, namely cooperation between ZIM and an HHU staff member who is the co-developer of eLabFTW and who already uses it at his institute.

4. Implementation

- ▶ Labfolder was introduced four to five years ago as a pilot project.

5. Current status

- ▶ Currently, between 60 and 100 researchers use Labfolder to document their research. The system is mainly used in the fields of chemistry and biology. New users can easily be created by ZIM in just “a few clicks”, with the licence costs passed on to the institute.
- ▶ Approx. five testers recently began testing the eLabFTW solution. eLabFTW is not discipline-specific. That means it can be used for any laboratory that keeps lab notebooks but does not provide any specific integration of other software or specific formula calculators. The system consists of blank pages that have to be structured by the user. The testers were asked to track their laboratory procedures in the ELN and assess how well this works and what problems arise. ZIM intends to further develop the open-source software if specific functionalities are needed.
- ▶ The company Labfolder offers free training for its system. No equivalent offer is provided with the open-source product. ZIM therefore intends to identify any training needs itself and develop whatever types of training may be necessary.
- ▶ An important topic at present is how to export data from the lab notebooks and transfer these data to the university's digital preservation system.

6. Lab system in the context of RDM

- ▶ The ZIM is collaborating with Wuppertal and Siegen universities to establish/improve research data management at the individual sites.
- ▶ Training courses on RDM also cover the topic of electronic lab notebooks. This topic is addressed on a site-specific basis in each case.
- ▶ The partners are currently establishing a university-wide repository at each of the three sites with a solid focus on facilitating the publication of research data, including DOI assignment. An electronic lab notebook can also be published in this way using its export function. It is not currently possible to automatically exchange data between an ELN and the repositories.
- ▶ Central data storage locations are being set up to increase resilience.

7. Summary

When operating several systems at the same time, it seems obvious that it should be possible to share data between the systems, e.g. from eLabFTW to Labfolder and vice versa. A standardised data exchange format would clearly be very helpful, but development of such a format is not really in the vendors' interests. A standardised format would only be offered as a feature if users were to rate this requirement as a key criterion for choosing which system to purchase.

8. Find out more

- ▶ Link to the ZIM: <https://www.fdm.hhu.de/en.html>
- ▶ eLabFTW resources:
 - Tutorials in the HHU Media Library:
 - <https://mediathek.hhu.de/watch/d6ab33ed-23d3-405a-b9fa-88bb1e02f5cd> (First steps, Video)
 - <https://mediathek.hhu.de/watch/15622584-635b-4c92-9171-30cbo98b26a> (Experiments & templates, video)
 - Links to further tutorials in the HHU Media Library
 - Virtual meeting of eLabFTW users on 2020-07-14:
 - <https://mediathek.hhu.de/watch/odcdd303-7fb1-4d58-b8c6-888398006ee1>(Video)
 - https://www.fdm.hhu.de/fileadmin/redaktion/Forschungsdatenmanagement/ELNHHU_Slides_Combined.pdf (slides)
 - Nicolas Carpi, Alexander Minges, Matthieu Piel: [eLabFTW: An open source laboratory notebook for research labs](#) *Journal of Open Source Software*, 2(12), 146, doi:10.21105/joss.00146
- ▶ Poster presentation
Nina Knipprath, Maurice Schleußinger, & Bert Zulauf (HHU Düsseldorf): [Elektronische Laborbücher für Hochschulen, 18.2.2019](#)
[ELNs for universities], Zenodo.
<http://doi.org/10.5281/zenodo.2571815>

4. How to introduce an electronic lab notebook

The process of choosing and introducing an electronic lab notebook depends very much on the specific circumstances of each particular research institute. We therefore recommend starting with an analysis of the current situation. This will lay the groundwork for the decisions that must be made in the selection process. This process typically yields a shortlist of one or more suitable options. However, it may also lead to the conclusion that none of the commercial tools are suitable for wide-scale introduction. This is particularly

common at large research institutions with a heterogeneous set of laboratories or with laboratories that have very specific requirements. In this situation, it often makes more sense to opt for an in-house or open-source solution.

It may emerge that the best approach is a combination of the two options: in other words, introducing a commercial product as well as an open-source solution for some specialised labs that they can tailor to their needs.



How to choose the right ELN

Joanna Loveluck (2020)

[Finding the Right Electronic Lab Notebook with the Corey Lab](#)

Spence, McCutcheon, Donaldson (2020):

[University of Glasgow Electronic Research Notebook Case Study](#)

Victoria Marmillod:

[2019 review of best electronic laboratory notebooks Labsexplorer.com](#), 2019, (sponsored by ELN vendors)

University of Utah library: Liste von ELNs:

<http://campusguides.lib.utah.edu/c.php?g=160435&p=1051495>

Roberta Kwok:

[How to pick an electronic laboratory notebook](#)

Nature, Jahrgang 560, 2018, Heft 7717, S. 296-270, DOI: 10.1038/d41586-018-05895-3

Peter Boogaard, Patrick Pijanowski:

[Electronic Laboratory Notebooks \(ELN\) Mean Many Things to Many People](#)

Laboratory Journal, 2012

Michael's Domain:

[Moving from Paper to Electronic Lab Notebooks](#)

International overviews of ELNs with regularly updated product comparisons:

University of Cambridge, The Gurdon Institute:

<https://www.gurdon.cam.ac.uk/institute-life/computing/elnguidance>

Harvard Medical School ELN Matrix

<https://datamanagement.hms.harvard.edu/electronic-lab-notebooks>

4.1. Choosing the right ELN

4.1.1. Analysing the current situation

The first step is to answer a series of questions from the following key areas:

Budget:

What financial resources are available to acquire and run an ELN? It is also important to plan for the cost of adapting a commercial product to your own needs in collaboration with the vendor. In the case of open-source products, additional funds may be required to hire external service providers if no in-house IT resources are available.

IT resources:

Do you have an IT department or staff with IT skills who can

- ▶ install and integrate the ELN into your IT infrastructure, e.g. by making a central storage location available?
- ▶ carry out ongoing maintenance such as updates and troubleshooting?
- ▶ develop the solution further and make any necessary changes?
- ▶ provide support?

What support is available for preparing training materials and information? Is there a library that can provide information, for example?

Current status in research groups/labs:

Are ELNs or “home-grown” solutions such as databases already being used? And do you intend to integrate these or migrate the data they contain into the new product?

Current status of research data management/IT infrastructure:


Are tools and infrastructure (hardware, software, central storage locations for research data) already in place? If so, which ones?

Analysis of the software environment:

Which existing software tools do you hope to use in combination with the ELN? (e.g. tools such as GraphPad Prism, FlowJo, ChemDraw, ChemDoodle, JupyterHub, Mind the Graph, LIMS)

4.1.2. Needs analysis and assessment

Users who will be working with the ELN might include researchers, laboratory experts, laboratory managers and IT administrators. Each set of users will have its own view on which requirements are most important. Features that are important to all groups include the ability to record essential lab-specific workflows and processes and fully document the research process.

The Needs Assessment  **Toolbox** contains a sample list of requirements. Needs assessments typically vary in scope depending on the initial situation, so some of the points in the list may not be relevant.

4.1.3. Criteria for selecting the best product

If you do not carry out a user needs assessment, the following criteria may help narrow down the choice. They can also be used in parallel with the needs assessment to help identify the most suitable products.



ELN workshops

Helmholtz open science workshop on electronic lab notebooks (2018):

Presentations in English:

OpenBIS (pdf):

https://os.helmholtz.de/fileadmin/user_upload/os.helmholtz.de/Workshops/elN18hzi_barillari.pdf

DotMatics ELN (pdf):

https://os.helmholtz.de/fileadmin/user_upload/os.helmholtz.de/Workshops/elN18hzi_wallace.pdf

Leibniz Association ELN Workshop 2018:

Presentation in English:

RSpace (pdf):

https://escience.aip.de/ak-forschungsdaten/wp-content/uploads/2018/11/20180612_RDM_ELN_RSpace.pdf

DH NRW/RWTH Aachen workshop 2017:

Presentations:

<https://rwth-aachen.sciebo.de/index.php/s/50C0ay7oc-j4w9be#pdfviewer>

Max Planck Digital Library ELN Workshop 2016:

Programm und Präsentationen:

https://eln.mpd.lmpg.de/?page_id=40





Literature on best practice examples

Stuart Macdonald, Rory Macneil:

[Service Integration to Enhance Research Data Management: RSpace Electronic Laboratory Notebook Case Study \(PDF\)](#),

DOI: 10.2218/ijdc.v10i1.354

Badiola, Bird, Brocklesby, Casson, Chapman, Coles, Cronshaw, Fisher, Frey, Gloria, Grossel, Hibbert, Knight, Mapp, Marazzi, Matthews, Milsted, Minns., Mueller, Murphy, Parkinson, Quinnell, Robinson, Robertson, Robins, Springate, Tizzard, Todd, Williamson, Willoughby, Yangd, Yllojaa

[Experiences with a researcher-centric ELN](#)

Chem. Sci., 2015, 6, 1614-1629, DOI: 10.1039/C4SC02128B

Pierre Tremouilhac, An Nguyen, Yu-Chieh Huang, Serhii Kotov, Dominic Sebastian Lütjohann, Florian Hübsch, Nicole Jung, Stefan Bräse:

[Chemotion ELN: an Open Source electronic lab notebook for chemists in academia.](#)

DOI: 10.1186/s13321-017-0240-0

Vaas, Witt, Windshügel, Bosin, Serra, Bruengger, Winterhalter, Gribbon, Levy-Petelinkar, Kohler:

[Electronic laboratory notebooks in a public-private partnership.](#)

DOI: 10.7717/peerj-cs.83

ELN concept:

- ▶ **Labs and researchers can be assigned to a single group with a specific focus (e.g. the life sciences):** Limit choice to ELNs that are particularly suitable for this group.
- ▶ **Labs and researchers can be assigned to one or more domains:** Limit choice to discipline-specific ELNs (e.g. for chemistry or biology).
- ▶ **Labs and research groups have a heterogeneous structure:** A generic, flexible and adaptable tool may be the most appropriate choice, possibly with a focus on specific disciplines.

Scope of ELN systems:

- ▶ The following types of systems are available:
 - "plain" ELN
 - ELN with LIMS (laboratory information management system), material management
 - data management platform/laboratory information system with ELN as a module

If other tools (e.g. a LIMS) are already in use, choose a plain ELN which can be connected to the existing software via standard interfaces or an API. Otherwise it may be worth choosing a product that also addresses other needs. Some LIMS solutions offer an ELN module, and vice versa. Comprehensive laboratory management systems are also available which include LIMS and ELN as modules. If further software is needed, purchasing a combined product can ensure all the modules work together seamlessly.

The distinction between ELN and LIMS is particularly important. An ELN is well suited to collecting diverse data in basic research, while a LIMS is used to collect highly structured data in analytical laboratories. Research projects usually generate unstructured, semi-structured and highly structured data, so a combination of LIMS and ELN may be a sensible choice. ^{xiv}

Price:


Some commercial vendors offer free versions for individual users and small research groups. However, in many cases these only offer limited features and/or limited storage capacity. These offerings are mostly based on the SaaS deployment model with cloud data storage. Some vendors

allow on-prem versions to be tested on request. For use in academic settings, they are usually offered at more moderate prices than for commercial use. Open-source products are available in their entirety free of charge.


→ [Find out more about deployment models/data](#)

Drawing on the experience of other research institutions

It may be helpful to identify which ELNs are already being used in equivalent areas of research at other institutions.

The  [infobox "ELN workshops"](#) provides a starting point with links to workshops where different approaches and products were presented.

It may also help to ask colleagues from other institutions the following questions: Where are you already using ELNs? What was the decision-making process like? What are your experiences so far?

Best practice examples can be equally helpful, some of which are included in this guide. Links to further examples can be found in the  [infobox "Literature on best practice examples"](#).

References provided by vendors can also offer information on sites where relevant ELNs are already in use

Invitation to tender:

After gathering all the relevant information, the next step is to prepare an invitation to tender to find the best product to meet your specific requirements. As our real-life examples have shown, relatively few vendors will actually submit bids on the basis of the tender, but those who do are likely to be offering ELNs that are genuinely suitable. This facilitates the decision-making process, though no ELN can be expected to meet every single requirement.

When preparing an invitation to tender, it may be helpful to examine invitations to tender issued by other organisations.

See the  [infobox "ELN tenders can provide useful input"](#).



ELN tenders can provide useful input

Examples of websites that publish invitations to tender:

Tenders Electronic Daily (EU):
<https://ted.europa.eu/TED/main/HomePage.do>

Opentender:
<https://opentender.eu/start>

Real-life examples:

Invitation to tender issued by Stockholm University (2020)
<https://ted.europa.eu/udl?uri=TE-D:NO-TICE:132754-2020-TEXT:EN:HTML&src=0>



BEST PRACTICE BOX

Case study: Robert Koch Institute (RKI) Berlin, LIMS with ELN functions developed in-house

Expert interviewed: Dr. Lei Mao, Department for Infectious Disease Epidemiology at the RKI, project manager and team leader for the in-house development of a laboratory system.

1. Background

- ▶ The RKI became aware of the need to deploy an electronic laboratory system about 20 years ago. It began taking concrete steps to select and introduce a laboratory system seven years ago.
- ▶ Most RKI labs have very specific requirements. They include national reference centres for pathogens and high-security biosafety level 4 labs. This means they generally have clearly defined workflows which a laboratory system would need to model.

Labs currently take heterogeneous approaches:

- Some of the labs use applications they have developed themselves, mostly Access databases. These work well but are not very user-friendly. Other disadvantages include a lack of interconnectedness and homogeneity (e.g. each lab uses its own layouts for reports).
- Many labs still use a paper lab notebook, mostly in hybrid form. In some cases, this involves significant extra work since figures and corrections must be entered into Excel tables on the computer as well as in the lab notebook. Some of the labs work with interim solutions such as OneNote and Filemaker, but these are regarded as too unwieldy and impractical for long-term use.

2. Needs analysis and cost-effectiveness study

- ▶ All the labs were asked to enter their needs and requirements (e.g. use cases, devices, essays, workflows) in a complex Excel spreadsheet. Evaluation of this spreadsheet revealed clear differences between individual labs. The RKI drew up an invitation to tender and tested some commercial products, but a cost-effectiveness study showed it would be too costly to adapt a commercial product to the different laboratories' requirements.

3. Decisive criteria for selecting a specific solution and key benefits

- ▶ Results of the needs analysis, tender and cost-effectiveness study.
- ▶ Developing a solution in-house keeps expertise and experience gained in-house.
- ▶ Preliminary steps already taken in-house can be used as a basis.
- ▶ Gradual implementation according to needs.
- ▶ Increase acceptance by offering users exactly the support they need.
- ▶ Efficient test phases thanks to internal communication and rapid communication channels.
- ▶ No need to rely on software vendor in terms of support, updates, proprietary formats, or specific hardware and environment specifications.

4. Implementation and planned scope

- ▶ **Personnel:** team consisting of project manager and three developers. One team member helped shape the upstream decision-making process.
- ▶ **Method:** agile software development with involvement of lab staff based on
 - user story workshops (definition of requirements),
 - task prioritisation, e.g. prompt implementation of very common lab methods such as PCR (polymerase chain reaction) and qPCR (quantitative real-time PCR) workflows,
 - and acceptance tests.
- ▶ **Scope:** the applications already used in the laboratories will be successively modernised, homogenised to the greatest possible degree, and connected together.

- ▶ **The following additional features are planned or already in progress:**
 - Audit compliance (for quality management tasks performed by accredited laboratories)
 - Ensuring evidentiary value: complete audit trail as per the German accreditation body DAkkS
 - Version management
 - Release attributes
 - Role management
 - Dashboard
 - Advanced search function
 - Inventory management (sample tracking, material database)
- ▶ **Prioritisation:** Implementation starts in the labs that are most motivated (largely due to QM requirements) and most open to change. For labs that are still working primarily with paper lab notebooks, the priority lies with those that are most ready to embark on digitisation. This will inevitably have the effect that others will want to follow suit once they see the considerable benefits of an electronic system.

5. Current status

- ▶ An initial prototype module was tested with test data in autumn 2018. A beta release was due to be released later that same month (October 2018) and tested with real-life data.
- ▶ Testing involved close collaboration between the test subjects and the development team. Up to five laboratory staff members tested the module in the presence of the programme developers, giving direct feedback on user-friendliness, problems encountered, usability and requests for improvement.

6. Lab system in the context of RDM

- ▶ The lab system is regarded as part of the RDM system. It is intended to assist in assigning metadata, primarily by describing sample attributes and documenting their whereabouts.
- ▶ Small files from the lab system are stored in an SQL database, large data sets are to be stored in openBIS via an interface.

- ▶ The use of openBIS as a repository is the focus of another project at the RKI. The process should be designed to enable the actual data to be made available from OpenBIS in the event of publication, The goal is to enrich relevant metadata with information from the lab system.

7. Summary

- ▶ The most significant and important aspect of the project has been the communication between the development team and the users. Although programming is complex, the availability of professional programming skills has made this go faster than expected. The key is to comprehend what is needed and develop an understanding of how work is carried out in each lab. Laboratory staff can help clarify which aspects of the procedures may be changed, and which must remain the same. This approach achieves high levels of acceptance and keeps obstacles to a minimum. A well-planned introductory process is essential. So too is intensive training and a willingness to listen to people's doubts and problems. This helps overcome the kind of gradual reluctance that can derail the entire process of introducing a new system.
- ▶ The decision to develop the software in-house was made on the basis of the highly specialist nature of the laboratories at the Robert Koch Institute. Other institutes may be better advised to purchase and adapt commercial or open-source products.
- ▶ Shaping the development of an electronic lab notebook is a challenge that requires plenty of communication and can ultimately help to forge better connections within an institution.

8. Further information

- ▶ Link to the RKI's Infectious Disease Data Science Unit in the Department of Infectious Disease Epidemiology: https://www.rki.de/DE/Content/Institut/OrgEinheiten/Abt3/FG31/FG31_node.html

4.2. Testing the selected products

Once one or more test candidates have been identified, the next step is to decide on the number and sequence of the products to be tested. Testing more than two or three ELN test candidates may be too time-consuming and complex. Superficial tests with test data are of limited value, but they can give an initial impression of the software, which may help to further narrow down the range of options.

Some manufacturers offer free trial access or free versions for individual users or small workgroups. These kinds of offers can be used for preliminary tests, though it is important to remember that these versions run in the vendor's cloud. If you have already selected a shortlist of products, a good option is to carry out in-depth testing using typical real-life use cases from the lab. This is a useful way to put performance and usability to the test.

It is helpful to ask test subjects to fill out a questionnaire. This makes it easier to record and evaluate test results.

Tips on creating a test questionnaire can be found in the  [infobox “Creating a test questionnaire”](#).



Creating a test questionnaire

ELN scorecard provided by Labfolder, an ELN vendor:
<https://www.labfolder.com/wp-content/uploads/2018/07/ELN-Scorecard.pdf> (PDF)

Bettina Laugwitz, Martin Schrepp, Theo Held:
[Construction and Evaluation of a User Experience Questionnaire Conference Paper, November 2008](#),
DOI: 10.1007/978-3-540-89350-9_6

4.3. Introducing your chosen ELN

Successfully introducing an ELN is heavily dependent on the support given to users. Preliminary training and training materials are usually provided by the vendor in the case of commercial products. If you opt for an open-source product, you will need to create the training materials and run the training courses in-house. Even with good training, questions and problems will inevitably arise when people start using the product. These need to be solved as quickly as possible, otherwise there is a risk that users will be too frustrated to continue. A major investment in training and support is required in the early stages, but it is also important to keep providing information in subsequent stages to tackle new issues and assist new users.



Examples of institutional information on ELNs and RDM

Berlin Institute of Health:
<https://www.bihealth.org/en/research/quest-center/service/eln>

ETH Zürich:
<https://documentation.library.ethz.ch/display/DD/Table+of+Content>

University of Wisconsin-Madison Libraries:
<https://eln.wisc.edu/>

University of Edinburgh:
<https://www.ed.ac.uk/information-services/research-support/research-data-service/during/open-research-tools/rspace-notebooks>

Useful measures include the following:

- ▶ Make training materials and FAQs available on the intranet if only intended for internal use, otherwise on the internet
- ▶ Designate a member of the test team as a key contact
- ▶ Hotline
- ▶ Monitoring during ongoing operation

See examples in the  [infobox “Examples of institutional information on ELNs and RDM”](#).

4.4. Legal framework: the staff council

This chapter is related to the situation in Germany, in particular North Rhine-Westphalia. On the assumption that legal framework conditions also have international significance, it is included here as a source of inspiration.

The staff council may have a right of co-determination in the introduction of software intended to monitor the behavior or performance of employees. Although the electronic laboratory notebook is not primarily intended to monitor employees, it is objectively suitable for monitoring employees, even if it is purchased for other purposes. It is irrelevant whether the intention is to monitor or not. ^{xv}

The federal personnel representation act (section 75, cases of full co-determination) and the co-determination laws of the individual federal states regulate whether the staff council has co-determination or participation rights. In addition to the legislation, there are relevant court rulings on this issue. ^{xvi} Since the laws of the individual federal states may differ on this issue, it should first be found out which regulation applies in the federal state in question. For example, the LPVG (state personnel representation act) for North Rhine-Westphalia regulates that the staff council has the right of co-determination (LPVG (NRW) §72 (3) 2 to 5).

The right of co-determination of the staff council means that it can not have an equal say in the introduction of an electronic laboratory notebook. In this respect, its opinion on the matter is more of an advisory nature.

If the staff council has a right of co-determination, it can have an equal say in the introduction of an electronic laboratory notebook. This means that the ELN can not be introduced until the approval of the staff council has been obtained. It is therefore essential to involve the council in the introduction process. It is advisable to involve the council as early as possible, i.e. in the best case scenario, information about the introduction of an ELN is communicated as soon as it is being considered.

In most cases, the staff council requires documents such as a data protection report as a basis for its decision-making. The dialog and information process as well as the procurement, creation and evaluation of documents should therefore be included in the schedule. For example, a data privacy opinion can only be prepared once it has been determined which software (in which data center/in which infrastructure environment) will be used.

A service agreement is not required by law, but is recommended because it creates clarity and legal certainty. It should be noted that the staff council also has co-determination rights here. If a service agreement already exists for the introduction of software, it can be expanded.

Another option is to develop a trust agreement on the use of an ELN together with the staff council. This can make clear that the use of an ELN must not be detrimental to employees or organizational measures (e.g., rights and role management). In an emergency, if it is not possible to obtain the approval of the staff council in any other way, technical measures (e.g., deactivation of features) can be considered.

Schedule

- ▶ Idea of introducing an ELN: information to the staff council
- ▶ Selection phase: information on process (e.g., selection criteria)
- ▶ Test phase: information about the selected software products and the test scenario to the staff council; communicate decision after evaluation of the tests
- ▶ Preparation for implementation:
 - obtain and submit documents necessary for the staff council to make a decision.
 - recommended: extension of an existing service agreement or drafting of a new one, alternatively: drafting of a trust agreement
 - after approval by the staff council: introduction of the software

Further information from practice can be found in the best practice examples of Leibniz Institute on Aging (FLI) and University of Cologne (UzK) under the point Implementation.



BEST PRACTICE BOX

Case study: University Medical Center Göttingen, UMG -
commercial product: RSpace -

Expert interviewed: Dr. Harald Kusch, Department of Medical Informatics at University Medical Center Göttingen

1. Background

- ▶ Impetus came from an infrastructure project carried out as a sub-project by the interdisciplinary Collaborative Research Centre 1002 at the German Research Foundation (DFG). The DFG experts recommended paying particular attention to electronic lab notebooks and their implementation in everyday clinical research.

2. Needs analysis and decision-making process

- ▶ Formed pilot group of four to five researchers from different working groups.
- ▶ Gathered input on selection criteria/requirements
 - from the pilot researchers taken from the various working groups.
 - from the heads of the working groups.
- ▶ Drew up a list of criteria from the IT perspective (software and hardware).
- ▶ Carried out an in-depth market analysis of a broad range of products from the commercial and open-source sectors. The results showed that none of the commercially available products matched the requirements perfectly.
- ▶ Weighted all the factors using a mathematical matrix to produce a score. eCat was the highest-scoring product.
- ▶ **eCat testing:** researchers in the pilot group tested the usability of the software in everyday clinical practice. The results showed that an electronic lab notebook is a useful resource and a productive documentation tool for some researchers, thus affirming the benefits of using an ELN in principle. However, the project remained at the pilot stage because the programme is not very user-friendly and requires in-depth training. It also lacks some important functionalities.

It gradually became clear that, at its current level of development, the software could not be successfully implemented throughout the organisation. Multiple options were discussed, including the possibility of switching to a different product.

- ▶ **Beta testing of follow-up product (RSpace):** in 2014, the follow-up product to eCat was made available to eCat customers in a beta version. The first short tutorials made it clear that RSpace had achieved a level of development that was suitable for an across-the-board roll-out.

3. Entscheidende Kriterien für die gewählte Lösung und Vorteile

- ▶ UMG does not have the capabilities to professionally develop an open-source solution. Equally, researchers in the clinical setting do not possess the expertise required to develop and expand an existing open-source product (with a few exceptions, such as physics). Furthermore, a lack of resources would make it difficult to realise vital core functions with an open-source solution.
- ▶ **Developing a solution in-house does not match the institute's philosophy:** there is a fundamental trend towards outsourcing to avoid utilising existing resources for technical implementation. The typical approach is to buy or re-use a commercially available product and then deal with the problems that arise from its use.
- ▶ RSpace no longer requires as much training as its predecessor, eCat.
- ▶ **Cooperation with the vendor:** RSpace beta testers can submit feature requests and core function requirements which will be implemented by the vendor during ongoing development of the software towards commercial maturity.

4. Implementation

- ▶ Developed required core functions in cooperation with the vendor (funded as part of infrastructure sub-project development):
 - **Connection of files or file systems:** established a central storage location for all the members of a working group. Avoided duplicate data storage and management by inserting links to stored files in the electronic lab notebook instead of importing them.
 - **Export functionality:** ability to export in various formats, both human-readable and machine-processable (e.g. XML) as well as formats suitable for digital preservation.
 - **Monitoring:** developed an in-depth questionnaire to ask the users about the strengths and weaknesses of the product during use.

5. Current status

- ▶ **Good productivity:** individual researchers regularly document their work in the electronic lab notebook. Larger working groups also use it to cooperate and share findings with each other.

Further requirements to be implemented in collaboration with the vendor:

- **Create archive packages:** the export function exports not only the selected ELN contents, but also the files it links to.
 - **Export capabilities link to campus repositories based on Dataverse and Zenodo:** export capabilities are not something that ELN vendors feel is particularly in their interest. Requesting such features from the vendor reinforces and supports active research data management.
 - **Expansion of API plus user support:** one important example is the ability to transfer data between the ELN and software products developed in-house.
- ▶ Use of funding to commission features and thus play a part in influencing software development.

6. Lab system in the context of RDM

- ▶ The topic of electronic lab notebooks was approached in the context of an infrastructure project. As well as focusing on features that matter to individual work groups, this also put a priority on global considerations, giving functions such as linking and exporting files the status of core functions.
- ▶ The electronic lab notebook is part of a central research data platform and is designed to interact with other elements. For example, links to an antibody catalogue ensure unambiguous referencing both in the ELN and the publications produced on that basis.
- ▶ Links to complex data types, which usually arise from complex workflows, are created in the ELN by means of persistent identifiers.
- ▶ API used to integrate the electronic lab notebook into the research data infrastructure.

7. Summary

When an ELN is introduced, it is unlikely to meet every single requirement. It is not possible to aim for a product that covers all evolving requirements, because the complexity of such a product would impair its usability and make maintenance difficult. The key is to determine which requirements are essential and where the limits of the selected application lie. A link to other software products is a fundamental prerequisite for exchanging data. The focus must therefore be on exporting data from the ELN in a structured way and creating programming interfaces to do this.

8. Further information

- ▶ Links to UMG:
- University Medical Center Göttingen, Medical Informatics:
<https://medizininformatik.umg.eu/en/research/>
 - Collaborative Research Centre 1002:
<https://medizininformatik.umg.eu/news-details/news-detail/detail/news/sonderforschungsbereich-herzschwaeche-verlaengerto/>
- ▶ Publications:
- **Kusch, Harald:** [Pilot integration of an electronic lab notebook and an Open Source research data repository as part of a modular biomedical research data platform](#), Göttingen Research Online, V1, 2018
Download (The PDF file contains the slides presented at the Dataverse Community Meeting in 2018, Harvard, MA, USA). DOI: 10.25625/ISPNW
 - **Kusch, Schmitt, Marzec, Nussbeck:** [Datenorganisation eines klinischen Sonderforschungsbereiches in einer integrierten, langfristigen verfügbaren Forschungsdatenplattform](#) [Organising the data of a Collaborative Research Centre in an integrated, permanently accessible research data platform], German Association for Medical Informatics, Biometry and Epidemiology (GMDS), 2015-09-06 – 09-09, Krefeld. Meeting Abstract DOI: 10.3205%2F15GMDS104
 - **Umbach, Freckmann, Knopp, Meyer, Suhr, Kusch:** [From seamless acquisition and sustainable management to publication of next-generation sequencing data](#)
German Association for Medical Informatics, Biometry and Epidemiology (GMDS), 2018-09-02 – 06, Osnabrück. Meeting Abstract DOI: 10.3205%2F18GMDS098

5. Categorisation of electronic lab notebooks

Methods of categorising electronic lab notebooks:

- ▶ **By features:** basic ELN, traditional ELN, high-end products ^{xvii}
- ▶ **By IT concept:** deployment model and data storage
- ▶ **By concept:** generic, generic with specific focus, discipline-specific ^{xviii}
- ▶ **By licence model:** commercial solution, open-source tools

5.1. Categorisation by features

Basic ELN or DIY solutions

This category comprises tools used as ELNs that were not originally developed for this purpose. Examples include Evernote, OneNote, OneDrive and Dropbox. These tools are inexpensive and easily accessible, and many researchers are already familiar with them. However, a disciplined and well-organised approach is required to adequately replicate the functions of an ELN with these tools. ^{xix}

This type of software is the closest equivalent to a paper lab notebook. In that sense, it is a good choice for making the switch to a digital method of documenting the research process.

However, it takes considerable effort to set up such a system in a way that covers the full range of functions of a traditional ELN. Such systems also have a number of other major disadvantages:

- ▶ Software updates are not always backwards-compatible.
- ▶ Versioning may not be feasible.
- ▶ It is important to check the privacy policies of these tool providers/vendors since they do not always allow for the protection of intellectual property. ^{xx}
- ▶ Some tools are only available as a cloud solution without the option of storing data locally.

Some traditional ELNs offer the ability to import data from such systems.

Traditional ELN

A traditional ELN is one that allows unstructured data entry (“just a blank piece of paper”) while also offering an extensive range of functionalities such as template options, sharing, compliance, input assistance, and so on. They also typically have an application programming interface (API).

High-end products

In this category of products, the ELN comes as a module of a comprehensive laboratory management system. Various combinations are available, including ELNs with LIMS and/or sample management, research data management systems that incorporate an ELN, and many others. See the [→ Scope of ELN systems](#) section in 4.1.3 to discover the benefits of these systems.

5.2. Categorisation by IT concept

Some vendors only provide their software as Software as a Service (SaaS) with cloud storage, while others also offer on-prem options for local installation. SaaS is usually tied to cloud storage, while on-prem versions allow data to be stored on the user’s own server. More details can be found in section 3 (“What should an ELN offer?”) under point 3.8:

[→ Deployment model/data storage.](#)

5.3. Categorisation by concept – generic, generic with specialist focus, discipline-specific

Generic ELNs are suitable for all fields of science, though some include a focus on a specific area, for example with special functionalities for chemistry or biology. Some are tailored to more specialised fields such as the life sciences, while discipline-specific ELNs are tailored to one specific discipline, offering features such as dedicated pre-configured templates.

5.4. Categorisation by licence model - commercial, open source

Most commercial ELNs use proprietary file formats to store data. The source code is almost always closed-source, i.e. it can only be modified and improved by the provider. Users are required to pay for a licence to use the products. Open-source products can be used free of charge. The source code is freely accessible and, in many cases, is actively developed by a developer community. Open-source products usually use open standard data formats.





BEST-PRACTICE-BOX

Case study: Cologne University and University Hospital Cologne

Commercial product: eLabJournal

Experts interviewed: Karin-Sylke Bartels, Stefan Schwenke

Karin-Sylke Bartels works at the University of Cologne's Regional Computing Centre (RRZK), where she is responsible for the IT infrastructure for CECAD (Cellular Stress Responses in Aging-Associated Diseases). Bartels was in charge of introducing the electronic lab notebook.

Stefan Schwenke is the IT coordinator at the Faculty of Medicine. He supported the introduction of the ELN by interfacing between the IT departments of Cologne University and University Hospital Cologne.

The two interviewees manage the ongoing operation of the system together with another colleague from the university's computer centre. They are responsible for configuration, organising training, and user management (e.g. creating new groups).

1. Background

- ▶ Various tools were examined and tested from 2015 onwards. This process was driven by Prof. Pasparakis and the deans of the Faculty of Medicine and the Faculty of Mathematics and Natural Sciences. The Department of Biology of the Faculty of Mathematics and Natural Sciences was also involved. Having the introduction and selection process embedded at such a high level was key to its success.

2. Needs analysis and decision-making process

- ▶ Following in-depth testing, a number of CECAD working groups preferred the eLabJournal product. The CECAD cluster of excellence is jointly supported by the Faculty of Mathematics and Natural Sciences and the Faculty of Medicine.
- ▶ Due to the high purchase price, a tender was issued in mid-2018. Only one vendor submitted a bid (Bio-ITech).

3. Decisive criteria for selecting a specific solution and key benefits

- ▶ For reasons of data security, a key criterion was the vendor's ISO 27001 certification.
- ▶ Equally decisive was the ability to maximise fail-safe, resilient operation by setting up a redundant system.
- ▶ An open-source product was out of the question, since this would not include the necessary vendor support for installation, training and other needs.
- ▶ The option of a cloud solution was excluded for data protection reasons.

4. Implementation

- ▶ In March 2019, a contract was signed between the Bio-ITech company (now part of the Eppendorf Group) and the Dean's Office of the Faculty of Mathematics and Natural Sciences at the University of Cologne, which is supported by the Institute of Biology.
- ▶ **The chosen solution was the "Scenario 3: Redundant Setup" specified by the vendor.** As the name suggests, the entire system is provided with redundancy. This means that
 - should one of the redundant components fail, no data will be lost and operation will continue uninterrupted,
 - availability of the electronic lab notebook is always guaranteed,
 - maintenance work can be carried out while the system is running.
- ▶ Due to data protection law, the decision was taken to carry out an on-prem installation of the system on local servers in the university's computer centre (with the support of the vendor). Tests were run to confirm the system was fail-safe (disaster case).
- ▶ **In addition to the software for the electronic lab notebook, the following software is used as an infrastructure:** Windows Server 2012 R for application servers and Internet Information Services (ISS 8.5), Windows Server 2016 for domain controllers, RRZK-AD infrastructure, CentOS 7 for keepalived, HAProxy, Apache HTTP Server, Lighttpd and Ubuntu 16 for database servers, Galera cluster for creating and managing a fail-safe database server network, plus back-ups via the IBM

Spectrum Protect platform, Maria DB, which are backed up to the RRZK MySQL backup, and other applications. A total of 12 virtual machines were set up as servers. This project was supported by staff from the Server Infrastructure, Network Infrastructure, and Customer Service & Web Support departments.

- ▶ Starting in September 2019, eLABJournal was introduced successively into the various working groups. Data was migrated from lab notebooks that were already in the vendor's cloud.
- ▶ The provider ran the initial training courses. Acceptance of the eLABJournal among the researchers was already high during these face-to-face sessions.
- ▶ Overall, the system was very well received. There were few queries on how to use the software.
- ▶ One of the biggest problems was getting clinical staff accustomed to using their university account instead of the usual hospital account, because only their university account could be used to log in.

Involvement of staff councils in the introduction of the electronic lab notebook

- ▶ Four staff councils were involved, namely the academic and non-academic staff councils of both Cologne University and University Hospital Cologne.
- ▶ Early involvement from the planning phase is recommended.
- ▶ **The following documents had to be submitted. They could only be created after a specific system had been chosen:**
 - Data protection report by the university's data protection officer (based on the computer centre's data security form)
 - Proof that procedures are in place for technical security aspects
- ▶ Once the staff council had agreed to the use of the ELN, it was added to the list of information and communication systems (ICT). This list is an annex to a framework service agreement on the use of electronic systems, which is part of the employment contract of staff at the University Hospital.
- ▶ The ELN must be signed off by the staff council before it can be put into operation.

5. Current status and development

- ▶ 500 licences are available, 250 each for biology and medicine. About 350 of these are currently in use. Licence numbers can be increased in blocks of 100.
- ▶ To train new working groups, the vendor's online training sessions were recorded and made available to the researchers. The Center for Molecular Medicine Cologne is planning on-site training sessions to support the introduction of eLABJournal. Requests to use eLABJournal have also been submitted by the chemistry and physics departments of the Faculty of Mathematics and Natural Sciences.
- ▶ The licence costs are covered by the Dean's Offices. RRZK staff costs have not yet been taken into account. There is currently a one-year option, after which an extension can be granted for a total of three years under the same conditions. After that point, a new contract must be negotiated.
- ▶ For data protection reasons, only basic research may be documented in eLABJournal. It is not permitted to document drug studies nor to store human data.
- ▶ The PIs (Principle Investigator/head of a working group) determine whether eLABJournal is to be used in their respective working group. PIs are created by the administrators with specified rights and are assigned the desired number of licences. The administrators themselves have no access to the content.
- ▶ The PIs or group members act as administrators of the respective work groups. They handle the configuration of the work group, for example by creating and inviting members and assigning rights within the group.

★ BEST PRACTICE BOX

Case study: Cologne University and University Hospital Cologne UzK
(Commercial product: eLabJournal)

6. Lab system in the context of research data management

- ▶ There are no plans to store large amounts of data in the system; currently the maximum size of files to be imported into the lab notebook is 20 MB. Options are available to create links to existing storage solutions.
- ▶ Members of the Faculty of Mathematics and Natural Sciences and the Faculty of Medicine can store and archive research data in the RRZK. This also applies to researchers from other faculties at the University of Cologne.
- ▶ The University Hospital's science network is planning to create a research data infrastructure with central storage unit, archive and repository components.

7. Summary

The introduction of eLabJournal as a joint project by the Faculty of Medicine and the Faculty of Mathematics and Natural Sciences was only possible thanks to significant support from the deans and the computer centre at Cologne University. Access statistics show that researchers are able to work with the electronic lab notebook in a fail-safe and mobile way even when faced with the challenges of the coronavirus pandemic.

8. Further information

- ▶ Related links:
 - CECAD IT services and data management:
<https://www.cecad.uni-koeln.de/about/management/cecad-it/>
 - IT coordination for research and teaching at the Faculty of Medicine:
<https://medfak.uni-koeln.de/service/it-services/it-koordination>



Toolbox: Needs assessment for an electronic lab notebook



1. Lab requirements

Requirement	yes	no	Notes/comments
I prefer a "blank page" with a basic editor for tables, texts, sketches (similar to a paper lab notebook)	<input type="checkbox"/>	<input type="checkbox"/>	
Ability to import data (e.g. MS Office; csv; pdf; graphics: jpg, tiff; audio files: mp3; video: mov, avi; barcodes)	<input type="checkbox"/>	<input type="checkbox"/>	Indicate any specific formats required
Ability to import and process special scientific formats (e.g. FASTA, dicom, Genbank, jdx, mol, fcs, data generated by measuring instruments)	<input type="checkbox"/>	<input type="checkbox"/>	Any other specific formats required?
Special data entry and processing aids (e.g. scientific calculator, formula editor, dictation devices, digital pen, animal module, antibodies module, plasmids module, strains and cells module)	<input type="checkbox"/>	<input type="checkbox"/>	If yes, which ones?
Ability to create your own templates (e.g. for standard operating procedures (SOPs) or protocols)	<input type="checkbox"/>	<input type="checkbox"/>	Provide more details if applicable
Ability to import templates or preconfigured templates (e.g. for sequence mapping and sharing, protocols/methods for biology, chemistry, medicine, translational research)	<input type="checkbox"/>	<input type="checkbox"/>	Provide more details if applicable, including file formats for im
Ability to export data (e.g. pdf, xml, html, Word, csv, zip)	<input type="checkbox"/>	<input type="checkbox"/>	Any other formats required?
(Graphical) representation of workflows, processes, projects	<input type="checkbox"/>	<input type="checkbox"/>	
Ability to create links to files outside the ELN (e.g. to avoid duplication of stored data, to show correlations)	<input type="checkbox"/>	<input type="checkbox"/>	
Sample management, creating material databases within the ELN	<input type="checkbox"/>	<input type="checkbox"/>	
Standard interfaces, e.g. connection to a laboratory information management system (LIMS) or other software (e.g. FlowJo, GraphPad Prism, ChemDoodle)	<input type="checkbox"/>	<input type="checkbox"/>	Including an existing LIMS or existing software?
Collaboration functions: individual users and groups, institution-wide, cross-institutional; release settings for data and results, role management, administrator rights	<input type="checkbox"/>	<input type="checkbox"/>	Describe required functions if applicable

The ELN must be able to document the following processes, SOPs and workflows:

2. Good research practice (GRP)

Requirement	yes	no	Notes/comments
Documentation and traceability in line with good research practice	<input type="checkbox"/>	<input type="checkbox"/>	Provide more details if applicable
Ability to search for keywords and experiments in the ELN using free text search, advanced search, database queries and special search queries (e.g. searches for chemical formulas and reactions)	<input type="checkbox"/>	<input type="checkbox"/>	Provide more details if applicable: what exactly is required?
Ability to ensure evidentiary value, e.g. audit trail, electronic signature and time stamp, FDA CFR 21 part 11	<input type="checkbox"/>	<input type="checkbox"/>	Provide more details if applicable
Special requirements for regulatory compliance, e.g. GxP, ISO, FERPA, HIPAA	<input type="checkbox"/>	<input type="checkbox"/>	Provide more details if applicable
Access (at least "read only") for a minimum of ten years	<input type="checkbox"/>	<input type="checkbox"/>	Provide more details if applicable

3. Connection to RDM system

Requirement	yes	no	Notes/comments
Support for assigning metadata, e.g. input masks	<input type="checkbox"/>	<input type="checkbox"/>	Provide more details if applicable
Automatic metadata harvesting, e.g. extraction from log files, export from Excel spreadsheets	<input type="checkbox"/>	<input type="checkbox"/>	Provide more details if applicable
Integration of controlled vocabularies	<input type="checkbox"/>	<input type="checkbox"/>	Provide more details if applicable
Ability to assign persistent identifiers, e.g. digital object identifier (DOI)	<input type="checkbox"/>	<input type="checkbox"/>	
AConnection to repositories, publishing platforms, file sharing services (e.g. Zenodo, Figshare, Dropbox, OneDrive, Google Docs, Mendeley)	<input type="checkbox"/>	<input type="checkbox"/>	Provide more details if applicable
Connection to digital preservation systems	<input type="checkbox"/>	<input type="checkbox"/>	Provide more details if applicable

4. IT and data security

Requirement	yes	no	Notes/comments
Sensitive data will be stored in the ELN, e.g. patient data	<input type="checkbox"/>	<input type="checkbox"/>	
Application programming interface (API)	<input type="checkbox"/>	<input type="checkbox"/>	Provide more details if applicable
Deployment model: installation on user's/institute's own server	<input type="checkbox"/>	<input type="checkbox"/>	
Data stored locally at the institute or in the institute's own cloud	<input type="checkbox"/>	<input type="checkbox"/>	
Web-based access, device-independent	<input type="checkbox"/>	<input type="checkbox"/>	
Exit strategies (outgoing migration), e.g. Oracle, SQL, pdf (where necessary with corresponding data), csv	<input type="checkbox"/>	<input type="checkbox"/>	Any other formats required?
Data migration from other systems (incoming migration), e.g. zip archives, Excel files, databases	<input type="checkbox"/>	<input type="checkbox"/>	Any other formats required?
Can be run on all operating systems (Unix, Linux, Windows, Android, iOS, MacOS)	<input type="checkbox"/>	<input type="checkbox"/>	Specific operating systems required?

5. Miscellaneous

Requirement	yes	no	Notes/comments
Classroom edition for teaching	<input type="checkbox"/>	<input type="checkbox"/>	
Default language/multi-language support	<input type="checkbox"/>	<input type="checkbox"/>	Language(s) required

The following aspects of introducing an ELN are particularly important to me:



Toolbox:
Checklist for selecting, testing and introducing an electronic lab notebook



Selection phase

Completed	Task	Notes/comments
	Draw up a budget (purchase costs, running costs, subsidies where applicable)	
	Check IT resources (in-house, external)	
	Check existing infrastructure (software and hardware, central storage locations)	
	Carry out needs assessment (labs, researchers, IT if applicable)	
	Analyse data workflows (complexity, consistency)	
	Review current documentation methods (e.g. hybrid/paper lab notebook, ELN, in-house solutions)	
	Identify criteria for product selection (e.g. concept, system scope)	
	Select ELNs for test phase	
	Communicate with staff council	

Testphase

Completed	Task	Notes/comments
	Assemble test team(s)	
	Select workflows/use cases	
	Prepare test questionnaire	
	Determine sequence of ELNs to be tested	
	Commission any product modifications that may be necessary (external/in-house)	

Implementation phase

Completed	Task	Notes/comments
	Review available training programmes (offered by ELN vendor or prepared in-house)	
	Check/create support services (intranet/internet/hotline/FAQ/key contacts)	
	Develop monitoring system (questionnaire to get feedback, change requests)	
	Plan roll-out (sequence of labs/research groups, schedule)	

6. Annex

Questions from interviews on which best practice examples were based

Questions on how it all started

1. What triggered your organization's interest in introducing an electronic lab notebook?

When was that?

Were there specific situations or individuals that provided the initial impetus?

What or who gave rise to that initial impetus?

Questions on the steps towards a solution

2. How did things develop? Who pushed the topic forward and what was the backdrop?

Was a needs assessment conducted, for example?

Who carried out that assessment?

What were the results? When was that?

3. What was the process of selecting eligible products?

Were specific criteria developed for that process?

Who developed the criteria? How? Which criteria were important?

4. Did your organisation consider developing a solution in-house? Or opting for an open-source solution?

Which were the decisive criteria for approval/rejection?

5. Were multiple selected products put through a test phase? How was that phase designed?

Who did the testing?

Did anybody support and supervise the tests? Who?

Who evaluated the tests? What were the results?

6. What were the key criteria that led to the selection of the final product?

Questions on implementation

7. What was the process of introducing the ELN? Who was involved?

How was the ELN implemented? By whom?

What obstacles still had to be overcome?

8. Were tools such as questionnaires and guidelines developed during the selection and implementation process?

Who developed them?

How useful do you consider those kinds of tools to be? Which ones specifically?

9. How do things stand at the moment?

How many users does the ELN currently have?

What challenges do users face in their everyday work with the ELN?

Where can potential users find information about the ELN?

Is there an in-house support service? What form does this take? Who is it offered/supervised by?

10. Is the ELN linked to other existing systems as part of a research data management system? For example, is it linked to systems for digital preservation/archiving or repositories, or are plans in place to do that?

Questions about the future

11. What developments lie ahead from your perspective?

What goals should be met next/in the future?

12. How would you sum things up so far?

What conclusions would you draw from the process so far?

What advice would you give to others?

7. References

- i. **Quality management re-visited: a reflective review and agenda for future research:** <https://www.sciencedirect.com/science/article/abs/pii/S0272696301000882> [retrieved on: 2021-02-16].
- ii. **Definition from Wikipedia** https://en.wikipedia.org/wiki/Agile_software_development [retrieved on: 2021-02-16].
- iii. **ZBW, GESIS & RatSWD (2015). Auffinden, Zitieren, Dokumentieren: Forschungsdaten in den Sozial- und Wirtschaftswissenschaften** [Find, cite, document: research data in the social and economic sciences], doi:10.4232/10.fisuzida2015.2, p. 21: Documenting data. [retrieved on: 2021-02-16].
- iv. **Franke, Michael; Weraach, Jalal; Haarländer, Markus (2017): Elektronische Laborbücher in der Max-Planck-Gesellschaft** [Electronic lab notebooks at the Max Planck Society], URL: https://www.mpg.de/10988930/jb_2017 [retrieved on: 2021-02-16].
- v. **Website of the German Federal Institute for Risk Assessment:** https://www.bfr.bund.de/en/glp_federal_bureau-1488.html [retrieved on: 2021-02-16].
- vi. **International Organization for Standardization:** <https://www.iso.org/home.html> [retrieved on: 2021-02-16].
- vii. **Definition from Wikipedia:** https://en.wikipedia.org/wiki/List_of_International_Organization_for_Standardization_standards [retrieved on: 2021-02-16].
- viii. **Johannes, P. C./Potthoff, J./Roßnagel, A./Neumair, B./Madiesh, M./Hackel, S.: Beweissicheres elektronisches Laborbuch: Anforderungen, Konzepte und Umsetzung zur langfristigen, beweiswerterhaltenden Archivierung elektronischer Forschungsdaten und -dokumentation** [Probative electronic lab notebook: requirements, concepts and implementation for long-term archival of electronic research data and documentation], NOMOS, Baden-Baden, 2013. Project description: <https://www.belab-forschung.de/en/projekt.html> [retrieved on: 2021-02-16]
- ix. **University of Kassel, Constitutionally Compatible Technology Design project group (provet);** URL: <http://www.uni-kassel.de/fb07/en/institutes/iwr/personen-fachgebiete/rossnagel-prof-dr/forschung/provet.html> [retrieved on: 2021-02-16].
- x. **Text: Prof. Dr. Christian Johner;** URL: <https://www.johner-institute.com/articles/regulatory-affairs/and-more/21-cfr-part-11/> [retrieved on: 2021-02-16].
- xi. **Illustration based on Johner, C. (2016): "Was sollte ein Audit-Trail enthalten?"** [What should an audit trail contain?], URL: <https://www.johner-institut.de/blog/wp-content/uploads/2016/06/Audit-Trail.jpg> [retrieved on: 2021-02-16].
- xii. **K. Chandrasekaran: Essentials of Cloud Computing**, CRC Press, chapter 4, Google Books: <https://books.google.de/books?id=-GhYBQAAQBAJ&pg=PP1&dq=deployment%20model%20cloud%20computing&hl=de&pg=PA46#v=onepage&q&f=false> [retrieved on: 2021-02-16].
- xiii. **Definition from Wikipedia:** https://en.wikipedia.org/wiki/Proprietary_software [retrieved on: 2021-02-16].
- xiv. **Dr. Manfred Göbl: LIMS and ELN, Pharm. Ind. 74, No. 1, 38–44 (2012).**
- xv. **Haufe.de: Mitbestimmung/Mitwirkung / 2.4.17 Einführung und Anwendung technischer Kontrolleinrichtungen:** https://www.haufe.de/oeffentlicher-dienst/tvoed-office-professional/mitbestimmungmitwirkung-2417-einfuehrung-und-anwendung-technischer-kontrolleinrichtungen_idesk_PI13994_HI1409399.html [retrieved on: 04.08.2020], German only.
- xvi. **Haufe.de: Mitbestimmung/Mitwirkung / 2.4.17 Einführung und Anwendung technischer Kontrolleinrichtungen:** https://www.haufe.de/oeffentlicher-dienst/tvoed-office-professional/mitbestimmungmitwirkung-2417-einfuehrung-und-anwendung-technischer-kontrolleinrichtungen_idesk_PI13994_HI1409399.html [retrieved on: 04.08.2020], German only.
- xvii. **Ulrich Dirnagl, Ingo Przesdzing: A pocket guide to electronic lab notebooks in the academic life sciences, 2016, doi: 10.12688/f1000research.7628.1** <https://f1000research.com/articles/5-2> [retrieved on: 2021-02-16].
- xviii. **Svetla Baykoucheva: Managing research data: electronic lab notebooks (ELNs). Managing Scientific Information and Research Data, chapter 9, Chandos Publishing, 2015, pages 85–96, ISBN 9780081001950,** <https://www.sciencedirect.com/science/article/pii/B9780081001950000093?via%3Dihub> [retrieved on: 2021-02-16].
- xix. **University of Cambridge, The Gurdon Institute: Electronic Lab Notebooks - for prospective users. Information for researchers who are interested in adopting an Electronic Lab Notebook system for documenting research and managing data.** <https://www.gurdon.cam.ac.uk/institute-life/computing/elnguidance> [retrieved on: 2021-02-16].
- xx. **Kanza, Samantha; Willoughby, Cerys; Gibbins, Nicholas; Whitby, Richard; Frey, Jeremy Graham; Erjavec, Jana et al. (2017): Electronic lab notebooks: can they replace paper?** In: Journal of cheminformatics 9 (1), p. 31. <https://jcheminf.biomedcentral.com/articles/10.1186/s13321-017-0221-3>, DOI: 10.1186/s13321-017-0221-3, [retrieved on: 2021-02-16]

