

# Chemotion Electronic Lab Notebook (ELN)

Research Data Management with Chemotion ELN and the extension LabIMotion ELN

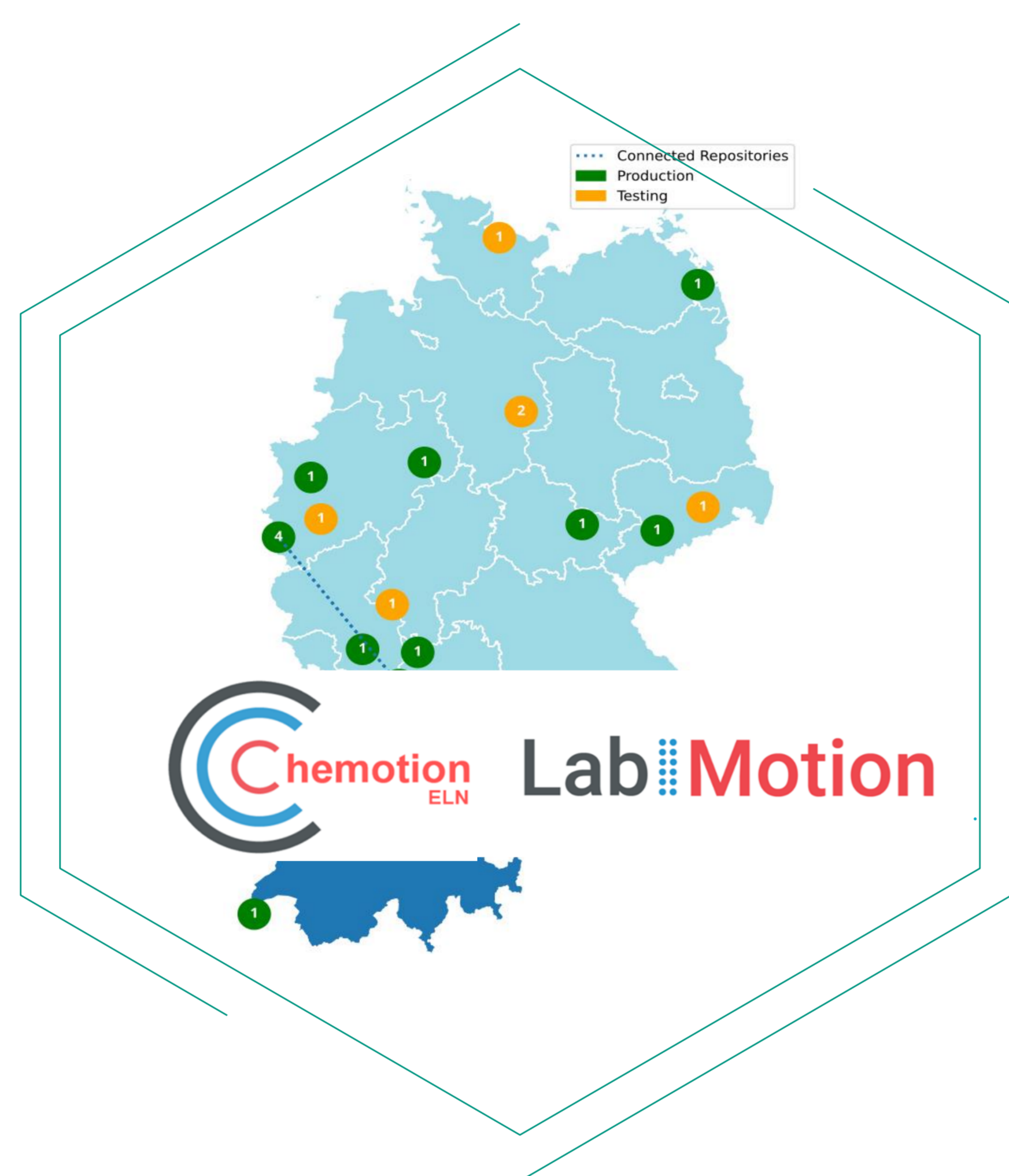
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## Chemotion Electronic Lab Notebook

Electronic Lab Notebooks (ELNs) are a key prerequisite to a comprehensive documentation of research processes, the digital storage of research data, and their reuse. ELNs can be used to plan, record, store and – in combination with repositories - disclose experiments or research data. In the long run, the benefit of ELNs is the option to store and manage data in a standardized way and to enrich the data with (automatically generated) information such as metadata, identifiers and descriptors. For scientists, ELNs offer advantages such as faster research processes and a faster access to information. Selected benefits of the ELN Chemotion - an ELN that was designed for the discipline Chemistry - will be presented to show exemplarily the use of research data management tools. The ELN offers special features for chemical work and includes diverse functions that allow the use of the ELN also in other disciplines. Both, the chemistry specific as well as the generic and adaptable modules will be presented in brief.

Chemotion ELN can be used in combination with the open access repository Chemotion. The disclosure of research data to the public is possible by a direct transfer of information from the ELN to the repository. The interoperable systems ELN and repository guarantee on the one hand an easy process for the disclosure of information and on the other hand the availability of comprehensive data including primary data and descriptions.

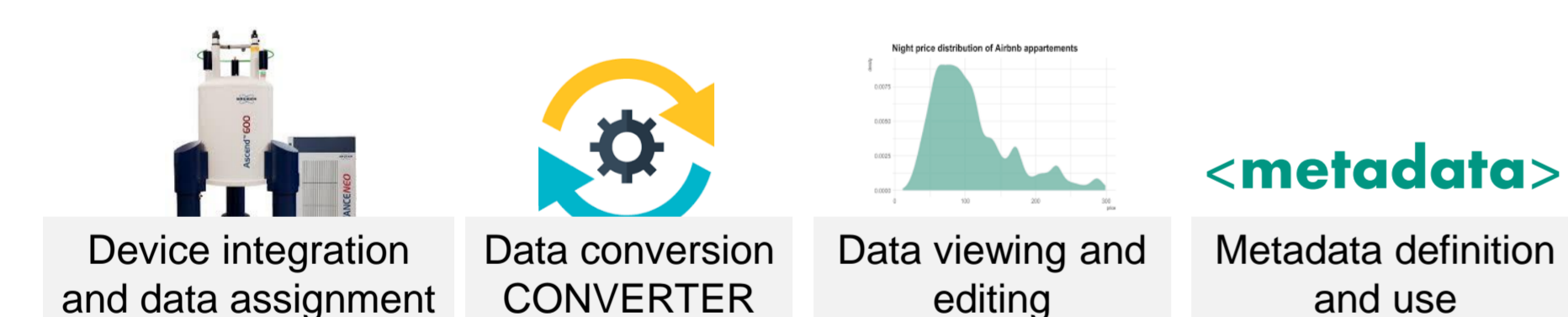
The systems Chemotion ELN and Chemotion Repository are part of the strategy of the National Research Data Infrastructure for Chemistry (NFDI4Chem) in Germany. The strategy and measures of NFDI4Chem will be described in brief.



## Basic components allowing the work with data

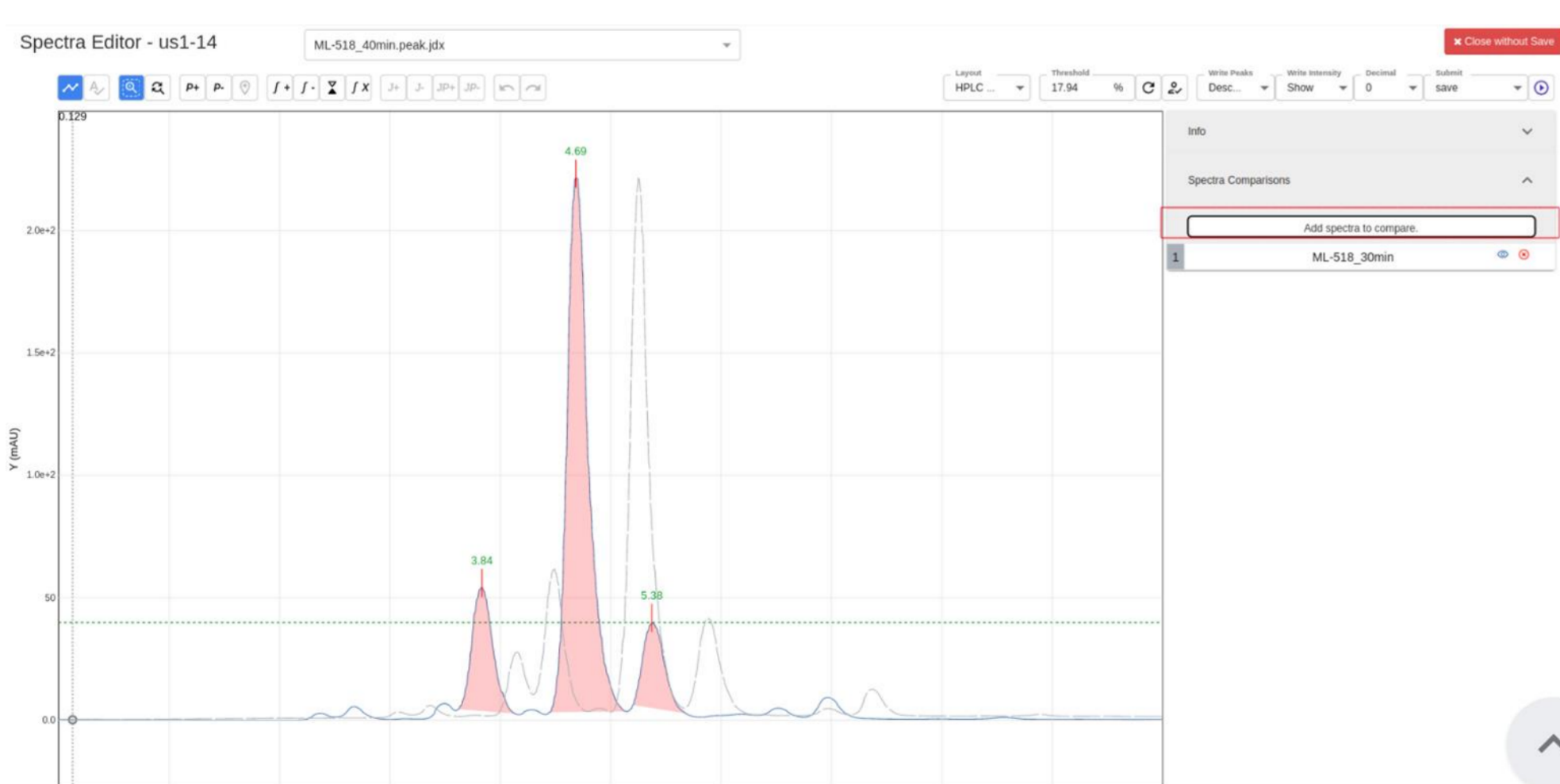
Chemotion includes a number of embedded software that supports the work with data. In particular the following four components are important:

- Device integration modules allow the transfer of data from devices to the ELN server
- Data conversion routines support the availability of standardized, readable and processable data
- Data viewers enable the analysis of data and their preview
- Metadata conversion routines provide discipline specific metadata



## Spectra viewer

Chemotion's spectra editor now supports editing and viewing data file formats for cyclic voltammetry, and HPLC UV-Vis measurements. Chemspectra can standardize supported file formats with the help of a converter service integrated into chemotion. This gives researchers more flexibility to process different types of raw data extracted from a wide range of spectroscopic measurements using the same spectra viewer.



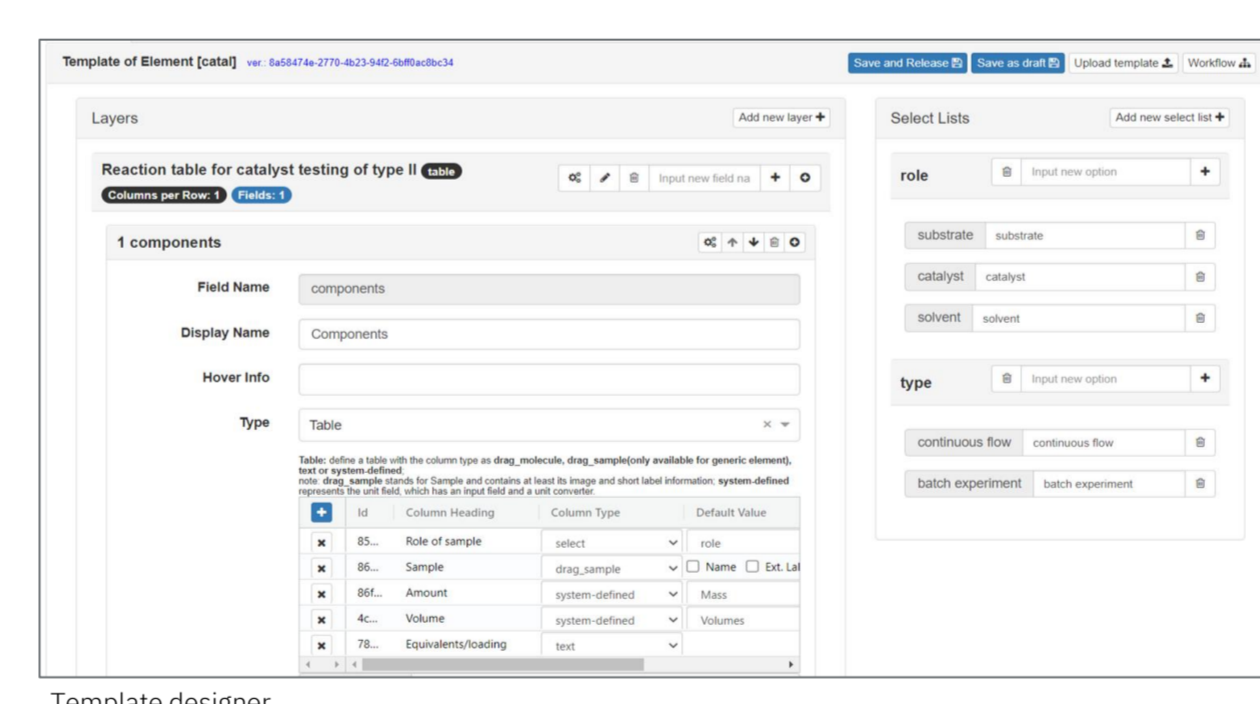
An example of the view of uv-vis spectra window in chemotion-ELN. Different spectra can be overlapped for comparison.

## Module design in LabIMotion

LabIMotion is an extension to Chemotion and -as Chemotion- a web application. With LabIMotion, scientists can build modules via the **Template Designer** and customise them to their needs, or get started by exploring the purpose-designed templates available in **Template Hub**. With this flexibility, LabIMotion is suitable as a research data management system for different scientific disciplines.



The **Template Designer** provides scientists with a variety of options to determine which kind of information to be displayed as ELN content and saved to the database. The designer also offers the option to set the layout of the defined metadata and to link the modules together, which makes LabIMotion suitable for a lot of complex use cases including related content. With the preview function, scientists can easily see the design template before it is released for use.



The **Template Hub** offers purpose-designed and reviewed templates, and they are open to the public. Scientists can browse the templates in the **Template Hub**, review the content of templates, retrieve what they need and start using them.

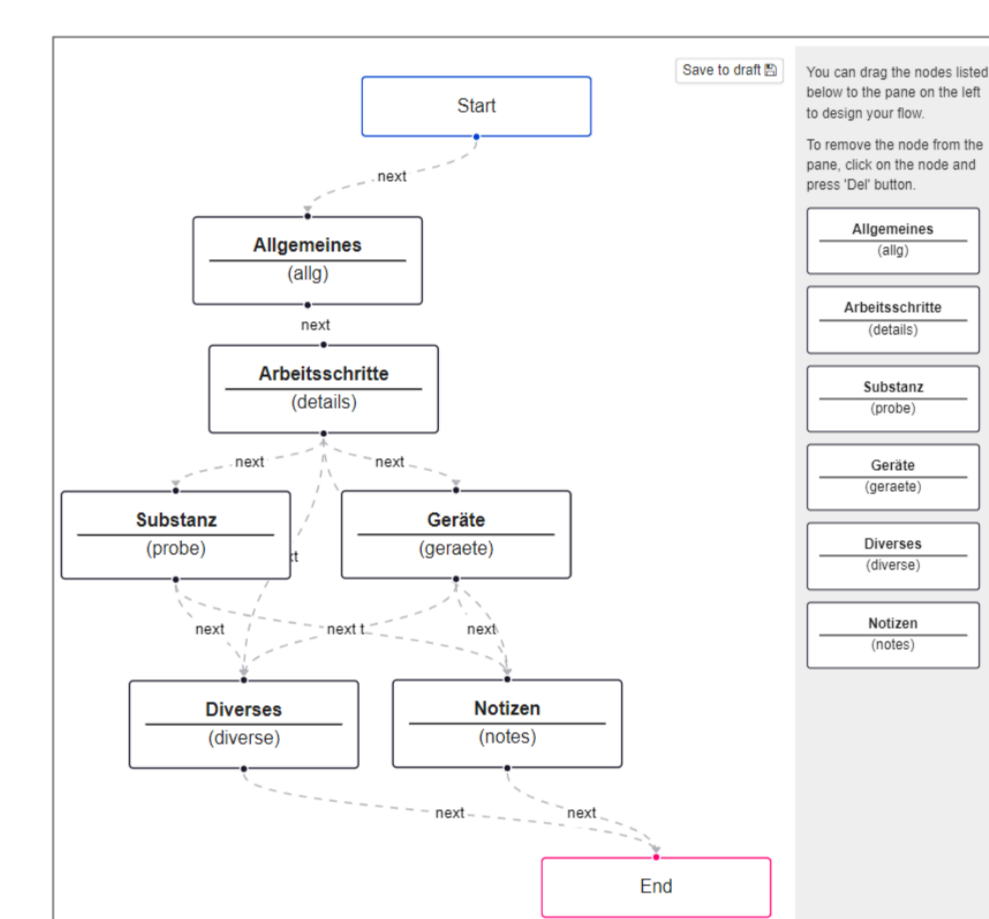
Segment Label	Description	Released at	Release to	Identifier
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MOF Segment	MOF Segment	13.07.2022 21:49	Sample	FAU2022-2406-4124-9862-02
MOF Reaction	MOF reaction	13.07.2022 21:48	Sample	FAU2022-2406-4124-9862-03
MOF Reaction	MOF reaction	13.07.2022 21:48	Sample	FAU2022-2406-4124-9862-04

**Chemotion ELN** is an Open Source lab notebook for chemists, including functions to acquire data, process data, and search data locally and in SciFinder and PubChem. It allows for advanced chemistry data management and sharing of the results with others.

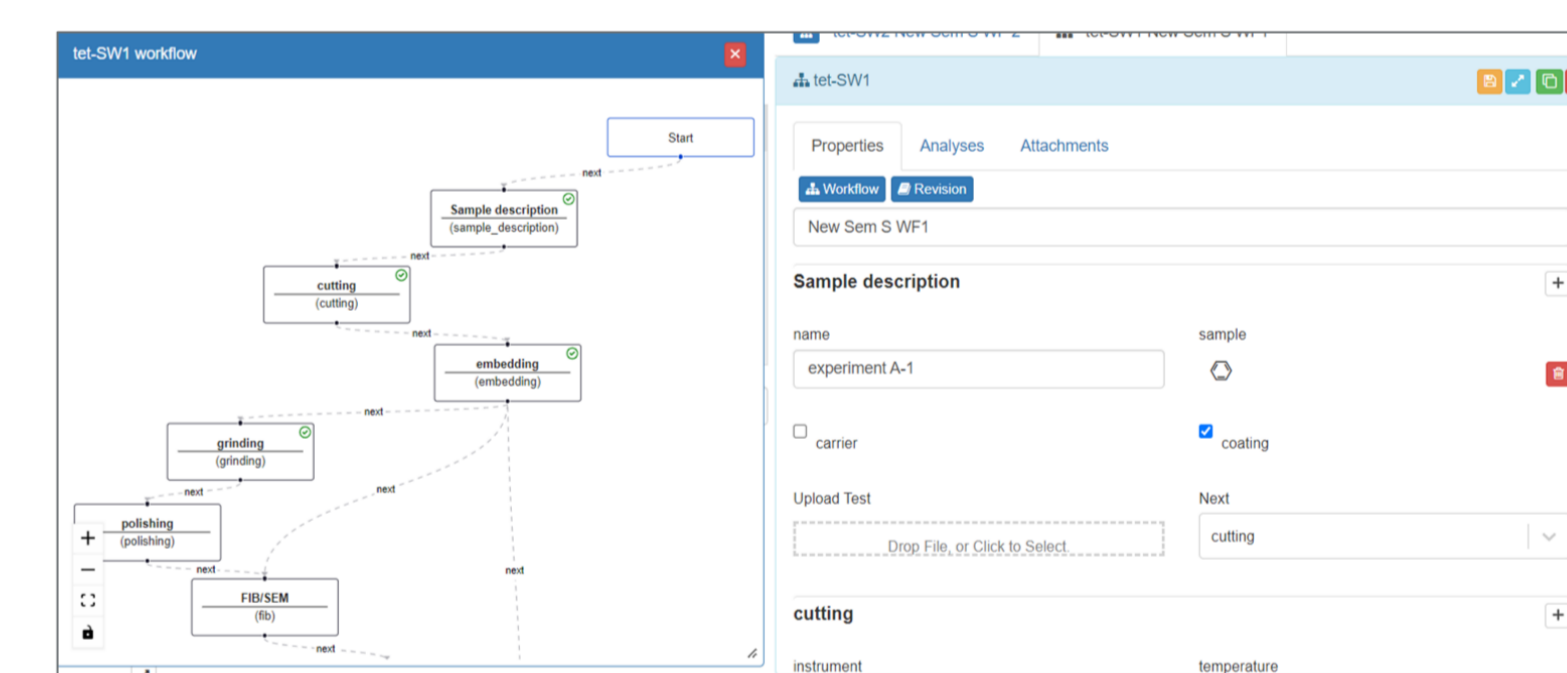
**LabIMotion** an extension of Chemotion ELN, that allows scientists to flexibly design new ELN modules. These modules can be interlinked to obtain a clear assignment of materials and samples in the processes and workflows.

## Process and Workflow

LabIMotion helps scientists to design new modules to meet their needs. In each module, scientists can define processes that include a series of actions/steps to achieve a result. It supports also to build workflow logics with interactive diagrams.



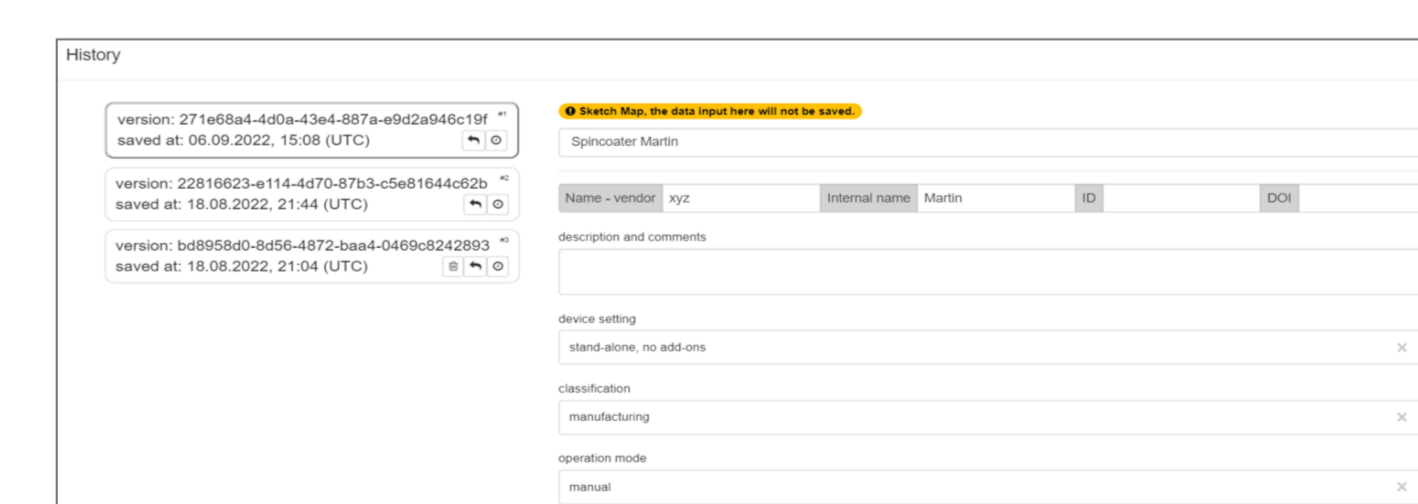
As a result, scientists can then focus on the most important parts with a clear view.



## Version history

LabIMotion maintains an automated revision history, which essentially means that scientists can go back to any version and restore it. Every revision made to the data is saved, which helps scientists keep track of changes to the content.

- **Revision:** Each time the content changes, LabIMotion creates a new revision history entry.
- **Review:** All revisions are listed in chronological order (from most recent to oldest). Scientists can browse different versions and review the content.
- **Restore:** By browsing different versions, scientists can easily access any version and revert to previous versions anytime.



## Current applications

Current applications: Polymer chemistry, MOF-segments, SEM/TEM preparations, device definition, measurement determination