Electronic Laboratory/Field Notebooks (ELN)

Marek Cebecauer

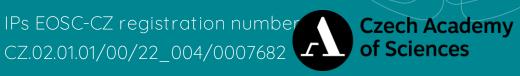
J. Heyrovsky Institute of Physical Chemistry

Czech Academy of Sciences







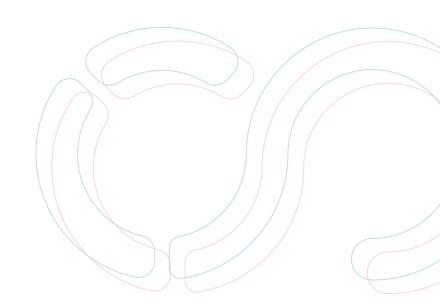






Outline

- What is an electronic laboratory/field notebook ELN?
- Why to use ELN?
- Which ELN is good for me?
- Comparison of selected ELNs
- Examples of use
- Questions/Discussion





Routine abbreviations

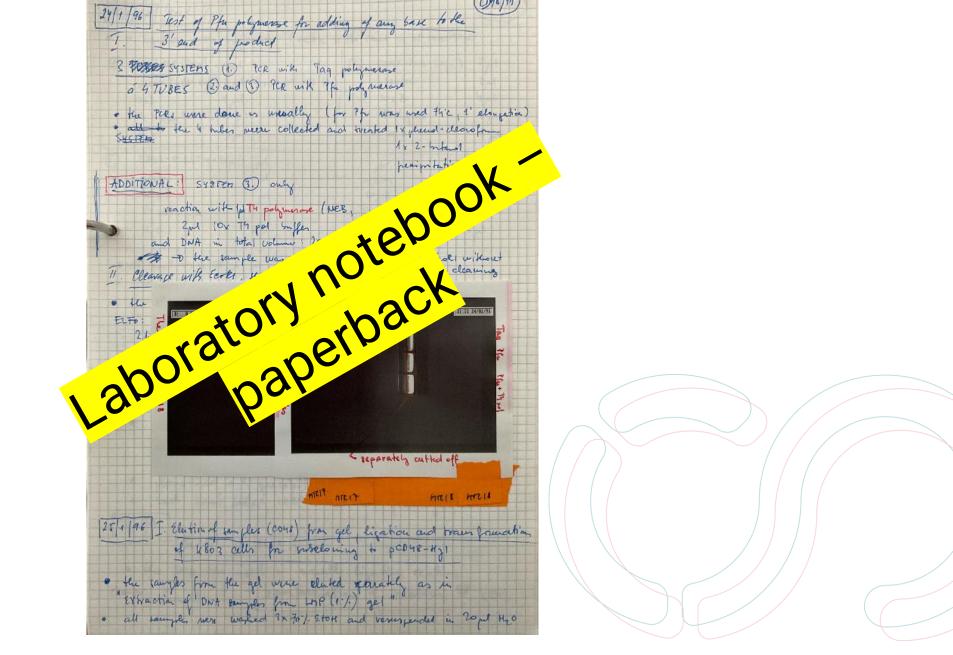
- Electronic laboratory (field) notebook (ELN)
- Laboratory Information Management System (LIMS)
- Research Data Management (RDM)
- National Repository Platform (NRP)
- FAIR principles Findable, accessible, interoperable, reusable
- Machine-actionable (MA)



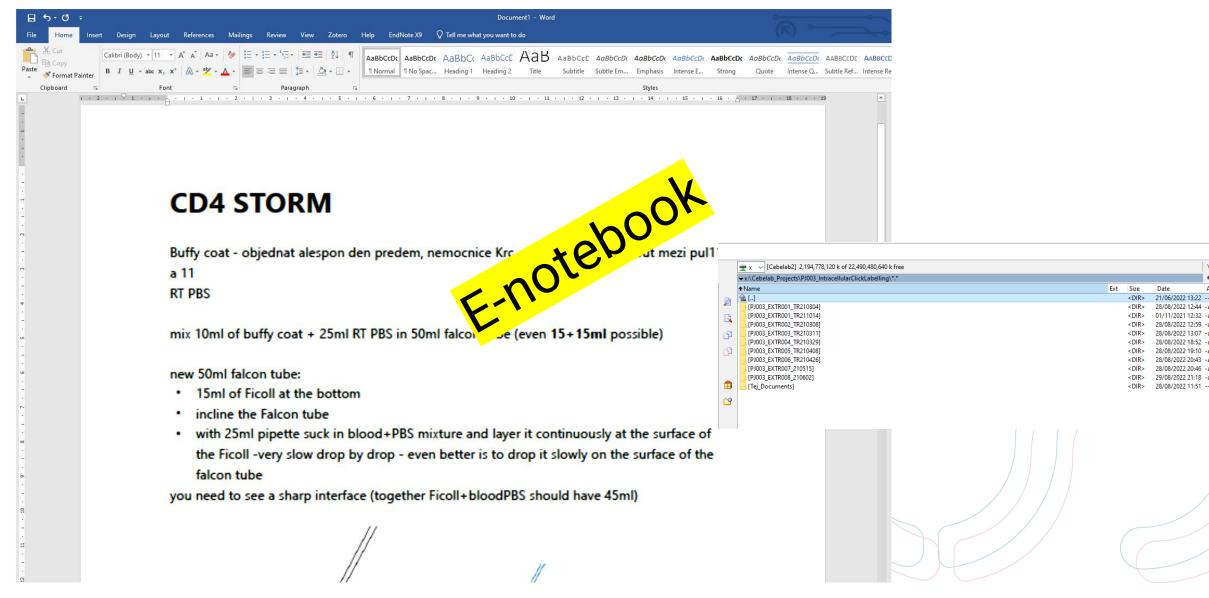
Scientific notebook styles

- Paperback notebook
- Electronic notebook (e-notebook)
- Electronic laboratory (field) notebook standard
- Electronic laboratory (field) notebook advanced
- Inventory / LIMS

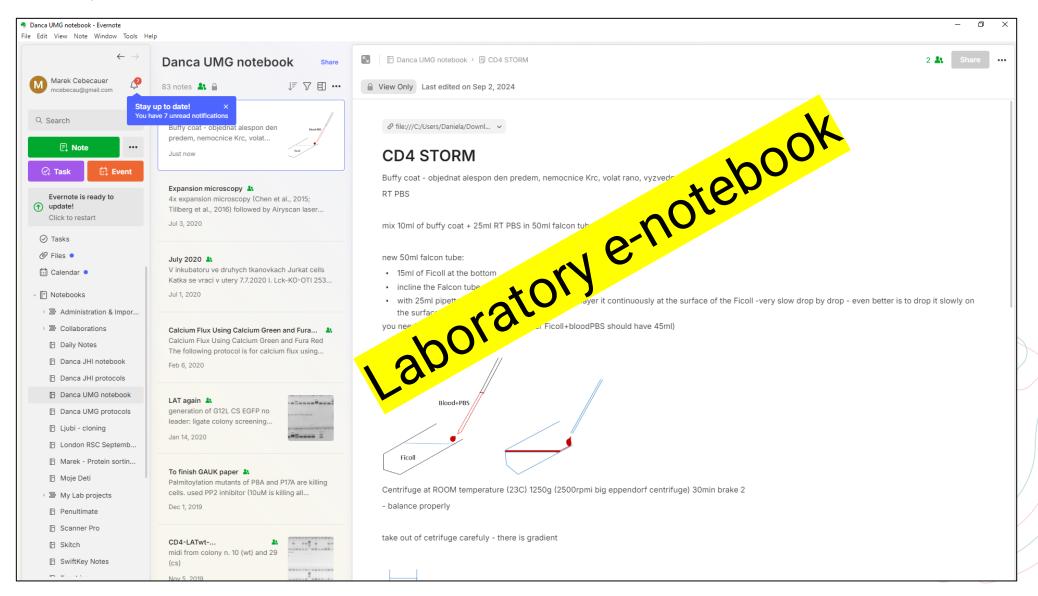




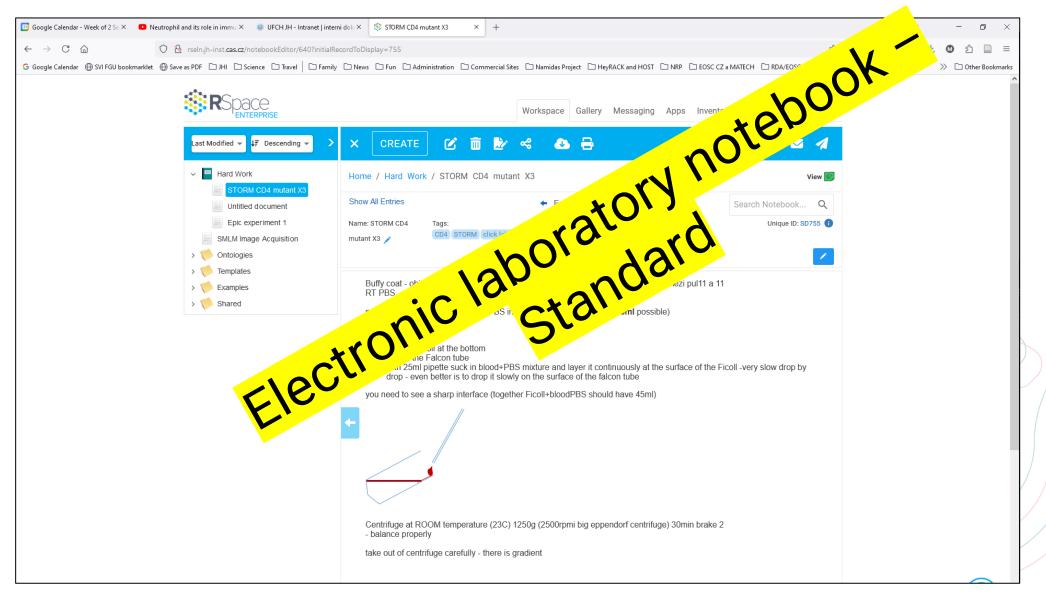




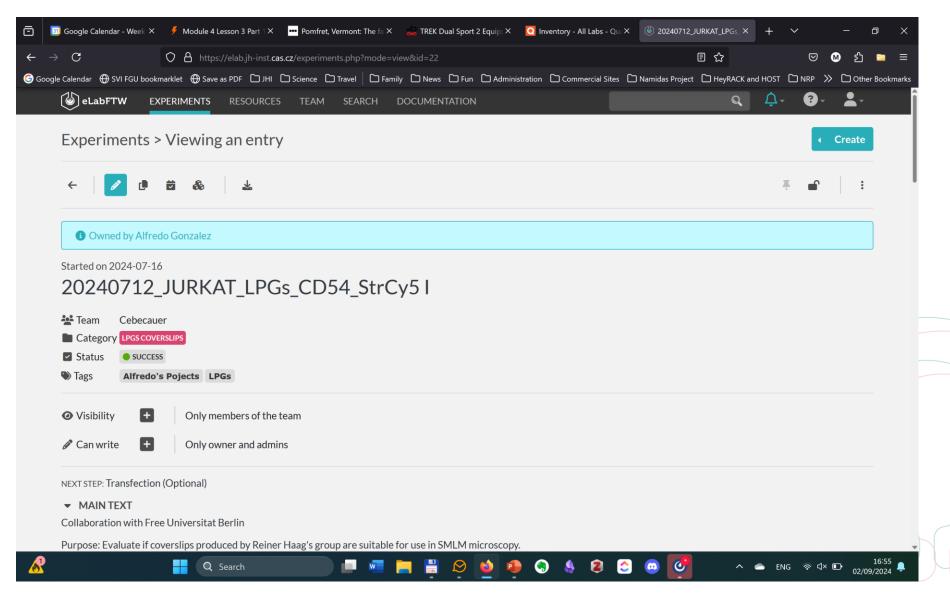




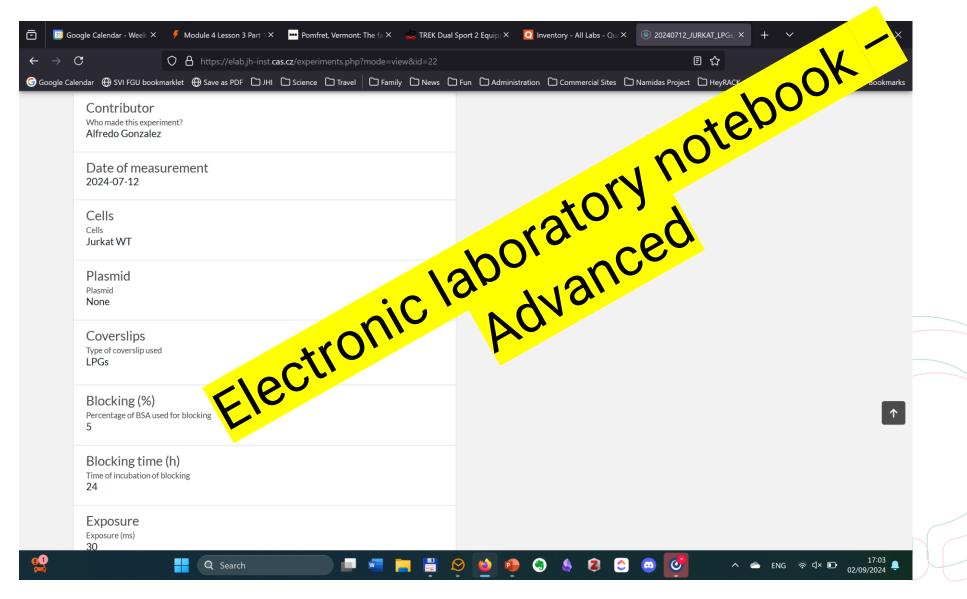




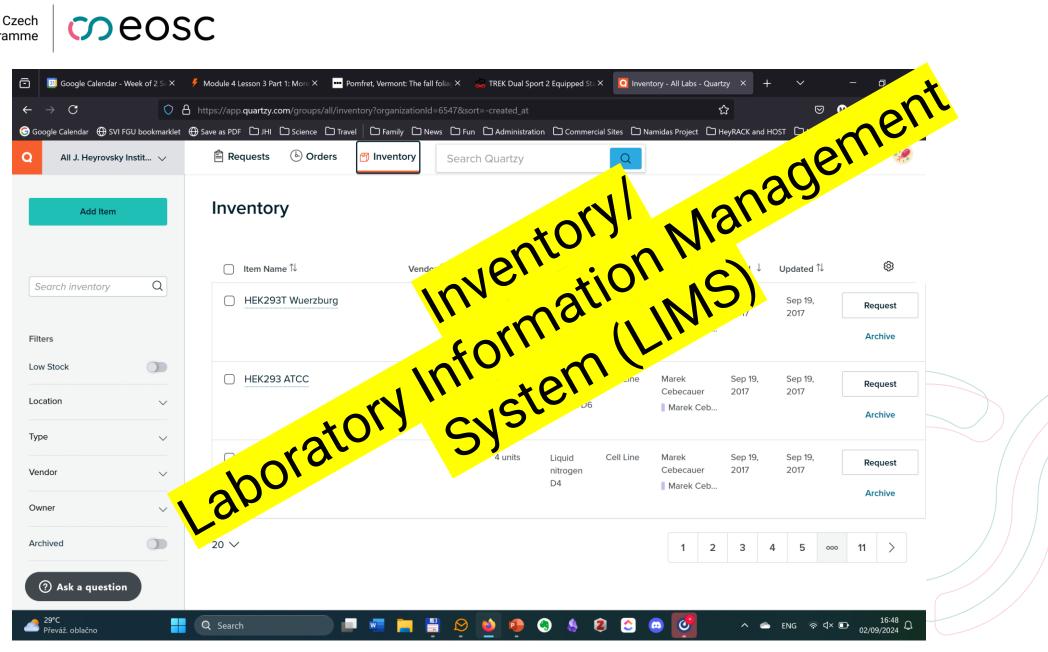












Scientific notebook styles

- Paperback notebook
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- Electronic laboratory (field) notebook standard
- Electronic laboratory (field) notebook advanced
- Inventory / LIMS



Harvard Medical School:

An Electronic Lab Notebook (ELN) is a software tool that in its most basic form replicates an interface much like a page in a paper lab notebook. In an ELN you can enter protocols, observations, notes, and other data using your computer or mobile device.



Imperial College London:

Lab notebooks are a way for researchers to remember vital information about their research through an organised and systematic manner. They may be considered part of your research data and will need to be archived along with your other data.



Imperial College London:

Easy, real-time collaboration and data sharing. Custom and template experiment records. Protocol library. Version-controlled repository (datasets) ...



Harvard Medical School:

Some ELNs can also manage inventories of samples, reagents, and other supplies, as well as keeping track of equipment and equipment maintenance schedules (LIMS functions). Additionally, some ELNs provide specialist scientific tools for chemical drawing or molecular biology.



Research.com:

An ELN can automate many of the manual elements of laboratory note-taking. In laboratory processes, automation simplifies experimental procedures and helps researchers save more time for other tasks such as data analysis. ELNs also use advanced technologies to automate different data input and acquisition processes.



Why to use ELN? ... Summary

- Records of experiments with relevant annotation and comments structured/templates/links
- Register of digital objects including digital representations of physical and abstract entities
- Versioning
- Access control to (meta)data. Collaborative functions.
- Protocols/procedures/workflows
- Links to the relevant data
- Optional: Data storage
- Optional: Inventory (samples, supplies, literature, data files)
- Optional: Instrument booking/scheduler
- Optional: Offline functions (electronic filed notebook)
- Optional: Timestamps (e.g., legal support)
- Optional: Signatures/witnesses
- Optional: Scientific tools (e.g. data visualisation, schemas)
- Optional: Automatisation of RDM processes





Why to use ELN? ... Summary







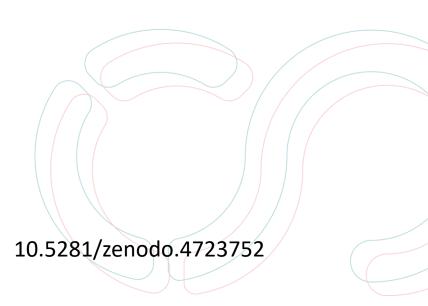
Which ELN?

- Avoid 'one size fits all' solution
- Personal preferences the principal investigator's (PI) responsibility
- Provide recommendations and support the PIs have to make the decision whether to use ELN or other tools.
- Offer more solutions (ideally diverse) for the RDM in your institution



120 ELN solutions (or more)

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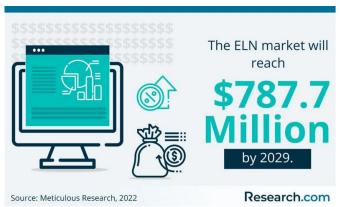




Find the right ELN for you.



https://eln-finder.ulb.tu-darmstadt.de/home



As much as of raw scientific data gathered in the 1990s have been lost. Source: The Availability of Research Data Declines Rapidly with Article Age, 2013 Research.com





RDM tool selection/Which ELN?

?

- Simple vs. complex
- Commercial vs. open-source
- Institutional instance vs. cloud version
- Does it support the export of FAIRified data?
- Sharing/collaborative options
- With LIMS vs. w/o LIMS (including scheduler and sample/equipment manager)
- Are specific scientific tools essential/needed?
- Integration with external scientific tools essential/needed?
- Is offline functionality essential/needed?
- Advanced functions: timestamping, signing, witnessing ... legal issues.



Selection of ELNs for NRP/MATECH

- From simple to more complex
- Open-source
- Institutional/national instances
- Must support the export of FAIRified and machine-actionable data?
- Sharing/collaborative options
- With LIMS and w/o LIMS
- Specific scientific tools: non-essential/favourable?
- Offline functionality: non-essential/favourable (expenses)?
- Optional: Advanced functions (timestamping, signing, witnessing ...)
- Automatisation processes: ready or not?
- Team of developers





Simple ELN for NRP/MATECH

- Basic functionalities: Records, Collections, Groups, Templates
- Open-source
- Easy to install and maintain institutional instances
- Supports the export of FAIRified/MA data: RO-Crate, RDF, JSON
- Sharing/collaborative options limited
- No extra LIMS functions
- No additional scientific tools: as off Sept 2024
- Offline functionality: NO
- Advanced functions: Publishing in ZENODO (simplistic version ⊕), workflows
- Prepared for automatisation: YES, advanced
- Prepared for integration with external scientific tools: YES, very advanced



Intermediate ELN for NRP/MATECH

- Basic functionalities: Projects, Experiments, Users, Protocols, Templates
- Open-source
- Standard installation and maintenance of institutional instances
- Supports the export of FAIRified/MA data: RO-Crate (ELN), JSON
- Sharing/collaborative options within an instance
- Limited LIMS functions, equipment registry and booking
- Specific scientific tools: drawing chemical structures
- Offline functionality: NO
- Advanced functions: scheduler (calendar), timestamping (legally: extra charge)
- Prepared for automatisation: Partially
- Prepared for integration with external scientific tools: Limited





Complex ELN for NRP/MATECH I.

- Functionalities: Spaces/users, Projects, Objects, Protocols, Publications, Templates
- Open-source
- Standard installation and maintenance of institutional instances
- Supports the export of FAIRified/MA data: JSON
- Sharing/collaborative options supported
- Advanced LIMS
- Specific scientific tools: molecular biology tools, big data, ...
- Offline functionality: NO
- Advanced functions: publish to ZENODO, scheduler (calendar), timestamping (extra charge)
- Prepared for automatisation: YES
- Prepared for integration with external scientific tools: YES, very advanced





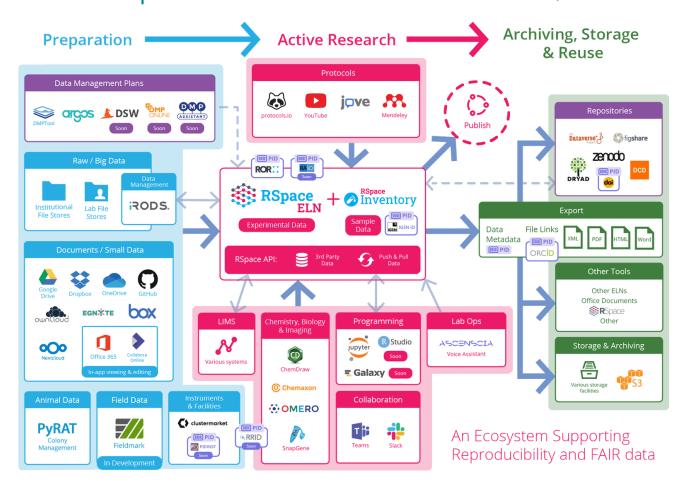
Complex ELN for NRP/MATECH II.

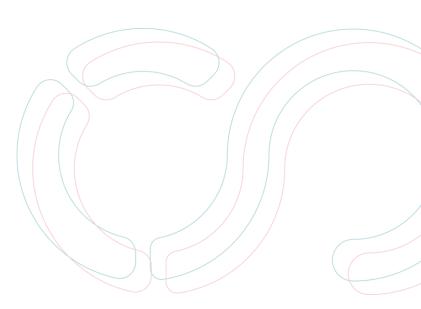
- Basic functionalities: Notebooks, Experiments, Users/Groups, Forms and Templates
- Open-source (from July 1, 2024)
- Standard installation and maintenance of institutional instances
- Supports the export of FAIRified/MA data: RO-Crate (ELN), XML
- Sharing/collaborative options within an instance
- Advanced LIMS, including IGSN registration
- Specific scientific tools: extensive integration with RDM tools, chemical structures
- Offline functionality: NO
- Advanced functions: scheduler (calendar), signing/witnessing, Dataverse and Protocols.io integration
- Prepared for automatisation: ??
- Prepared for integration with external scientific tools: YES



RSpace

Complex ELN for NRP/MATECH II.







Common features

- Creation of user groups and projects
- Access control (individual experiments, collections, (meta)data)
- Mandatory*/Recommended metadata fields
- A panel formats of metadata export (including human and machine-readable formats (PDF, XML, JSON, RDF)
- Customisable templates
- Python scripts/APIs



Distinguishing features – focusing on

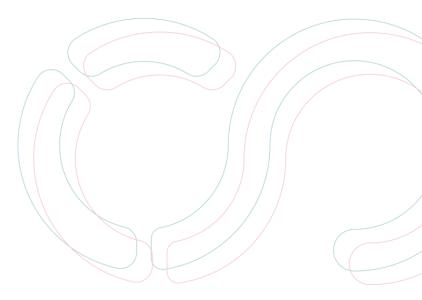
?

- Kadi4Mat: simple, workflows
- eLabFTW: protocols, scheduler
- RSpace: sample management/EOSC integration
- openBIS: professional RDM tool, domain-specific tools

FAIMS3/Fieldmark: electronic field notebook – offline functionality



ELN in praxis

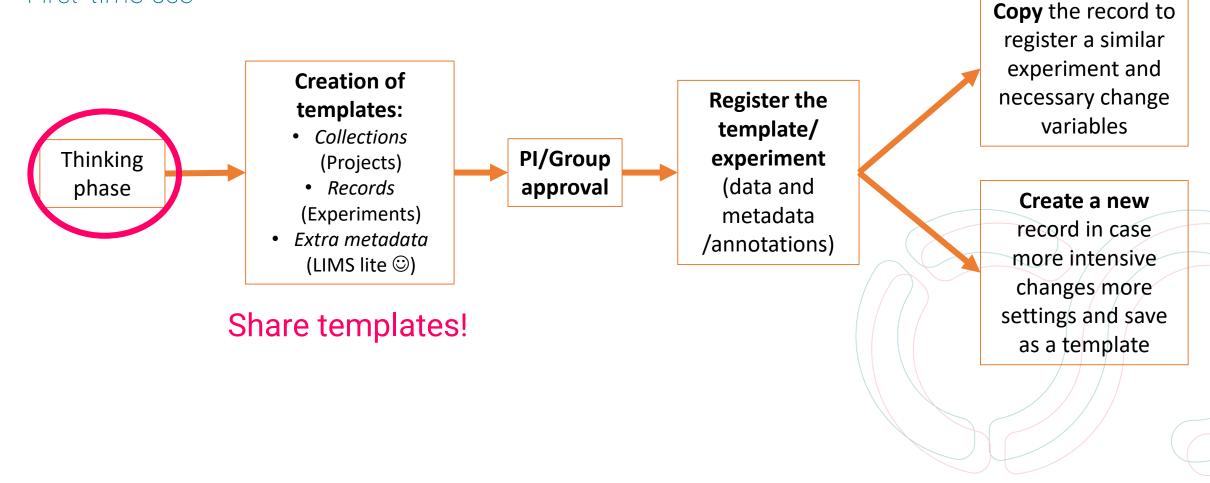






How to use ELNs?

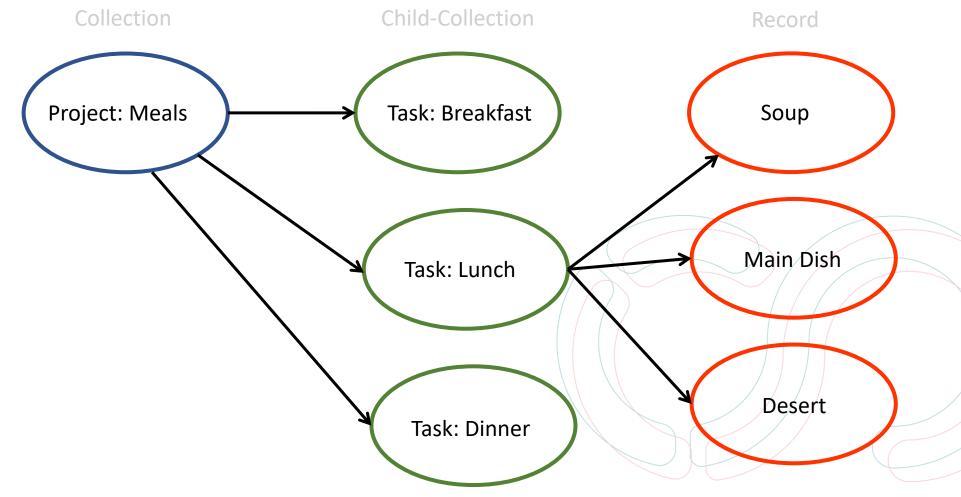
First-time use





How to use ELNs?

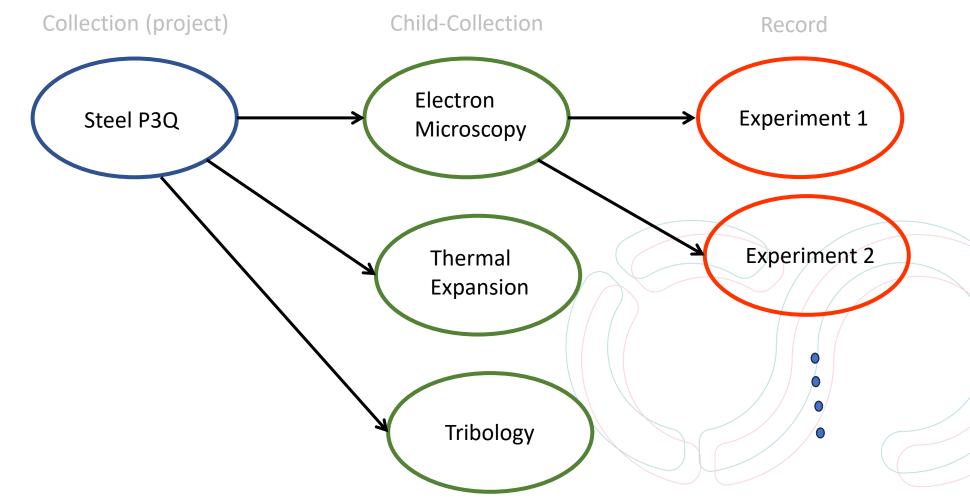
Structure of my project





How to use ELNs?

Structure of my project





Fields in the record - metadata schema

Mandatory

Recommended

Creator

Creator ID

..... ORCiD

Owner

Owner ID

..... ROR

Date

..... Date of the measurement

Sample

Sample ID

..... IGSN

Instrument

..... Select from the list

Instrument ID

..... PIDINST

Temperature

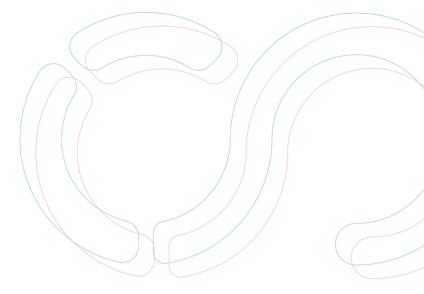
..... Integer: range 200-400 K

Pressure

..... Integer: value



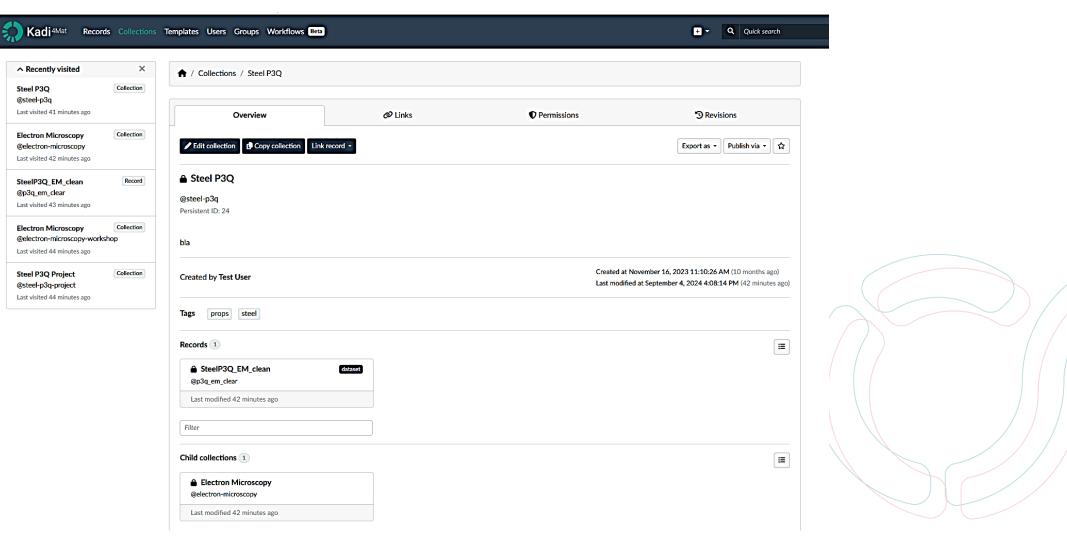
Live demo







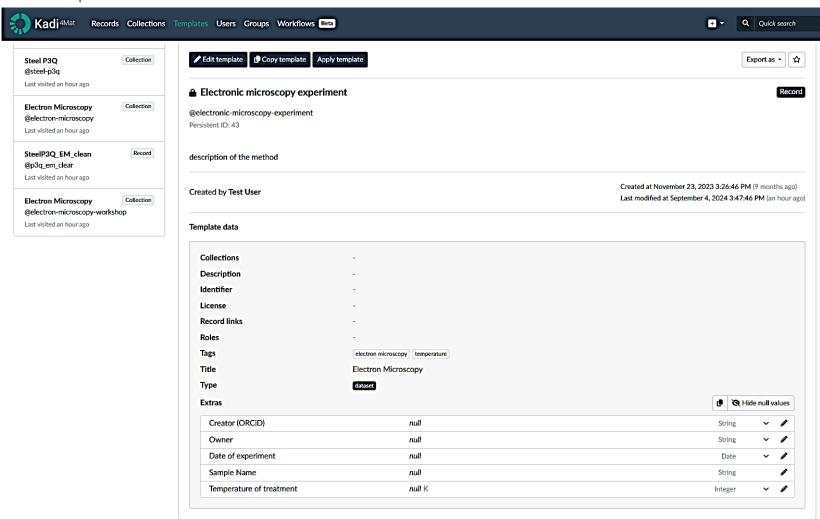
Collection

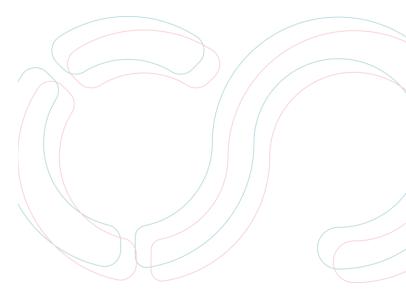






Template

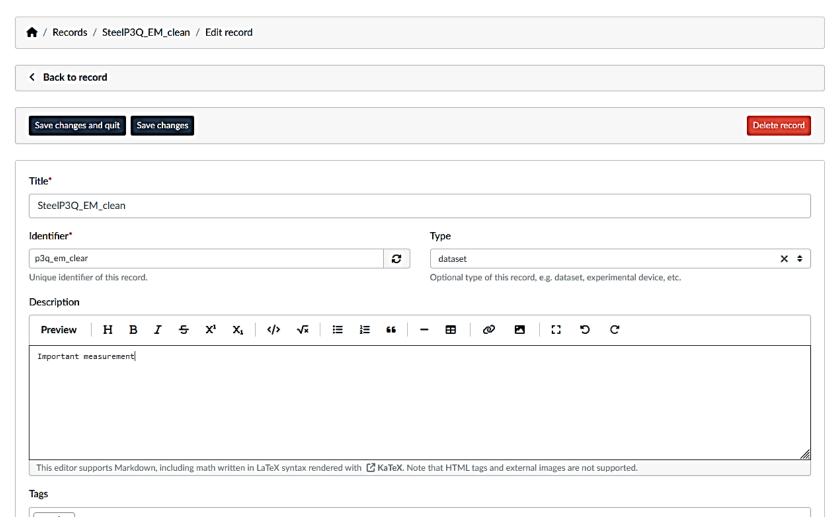


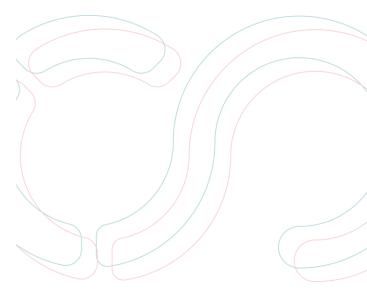






Record

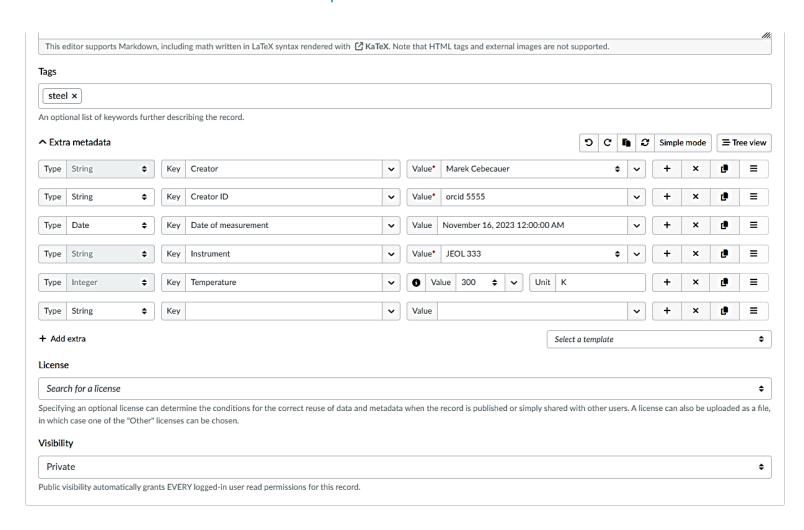


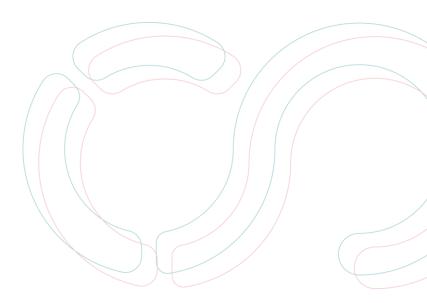






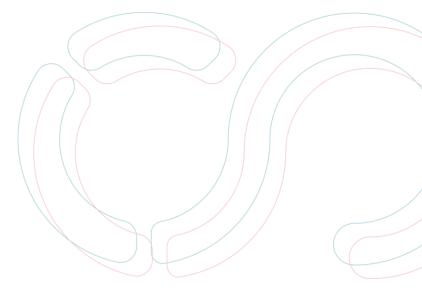
Record - from template







Discussion



Thank you for your attention.

marek.cebecauer@jh-inst.cas.cz







