

Facilitating Digitisation and Standardisation in Electrochemical Research through ELN Implementation and Template Development: A Use Case from a Data Steward Perspective

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The digitisation of laboratory workflows brings both opportunities and challenges, particularly in the area of standardised documentation and data management. In the field of electrochemical research, where precision and reproducibility are essential, the lack of standardisation of data documentation significantly affects the efficiency and reliability of research results. This presentation describes the journey of implementing the Chemotion Electronic Laboratory Notebook (ELN) in an electrochemistry research group and highlights the role of the research data management (RDM) support staff in facilitating this transformative process.

Initiation Process and Challenges: The initiation of this transformation came from the research group's strong interest in digitising their laboratory workflows with a view to open research practices, internal standardisation of research data management (RDM) and the development of standard operating procedures (SOPs). A comprehensive needs assessment led to the selection of Chemotion ELN, recognised for its chemistry-specific functionality and its adaptability provided with the LabIMotion generic extension to develop customised documentation templates. The challenge was, firstly, to become familiar with the ELN and its functionalities itself and, secondly, to accurately represent complex laboratory processes within it, given the limitations of available documentation templates for electrochemical research in the ELN.

Solution Development and Collaboration: It was essential for this project to first analyse and structure the laboratory processes to develop a concept for the creation of the templates. At the same time, extensive literature research was carried out on existing documentation recommendations, which were also considered in the templates. Using the LabIMotion extension of the Chemotion ELN, templates for the documentation and data collection of various sub-processes were then created and optimised in terms of structure, content and design using a dynamic and iterative feedback loop. As a result, three comprehensive generic elements and one generic segment were created to reflect the workflow in this electrochemical research area. There was also close collaboration with the ELN developers, where bug reports and feature requests were discussed and subsequently incorporated into new software versions.

Implementation and Community Engagement: The gradual introduction of Chemotion ELN, initiated with a test phase involving a small subgroup of the research team, before extending to the entire group, underscores the importance of a phased approach to technology adoption in research settings. The project aims to go beyond a single research group and contribute to the wider research community. By providing the templates to an expert review process and subsequent provision via the LabIMotion Template Hub, the initiative aims to encourage the reuse and adaptation of this best practice across electrochemical research. In addition, the provision of field names and descriptions, including relevant ontologies where possible, should enable wider applicability across different ELN platforms and documentation workflows.

The implementation of Chemotion ELN in an electrochemistry research group, led by the dedicated support of the research data management staff in all phases, exemplifies a successful model for digital transformation in the laboratory. Through careful planning, collaboration with software developers and community engagement, the initiative is not only streamlining the group's data management practices but also sets a best practice for standardisation and open research in the wider scientific community.

Abstract

Talk

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