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Systematizing experimental work by a template for electronic laboratory notebooks

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Highlights

- The general structure of scientific experimental work was abstracted, and the necessary steps highlighted.
- A structured framework to facilitate planning and execution of laboratory work by supporting the scientific thought process was developed in an ELN environment.
- The resulting template is shared to enable further use and adaptation, together with a commented example.

1. Introduction

Science relies on "quality"[1] for the essential qualities that have led to its success: reproducibility, predictability, falsifiability. Careful experimentation can be very time-consuming. In today's team-based working environment, it is therefore valuable to share work approaches openly and consistently to maximize effectiveness and minimize misunderstandings.

Electronic laboratory notebooks (ELNs) have recently soared in popularity.[2] Prior contributions in this area have focused on procedural, hardware and information technology aspects.[3,4] In addition to practical benefits (storage, sharability, and integration), ELNs offer an opportunity to structure thought. Accordingly, a systematic framework was created and embedded in Syngenta's ELN. This article shares the methodology and template so as to enable adaptations and improvements.

2. Methods

The framework was developed with the assumptions of Table 1 in mind.

Philosophical considerations	The most general science is hypothesis driven. Scientific abstraction requires interpretation to be useful. A clear purpose optimizes the benefit of work.
Practical considerations	The framework must encourage discussion between several parties - by explicitly listing assumptions and approach is beneficial. A highly structured approach induces clarity of thought. Efficiency is a key driver, leading to advance planning

Table 1. Assumptions for template development.

These principles led to the general framework in Figure 1. Syngenta uses the "Electronic Laboratory Notebook" from Dassault Systèmes. A special tab was added, which by procedure must be discussed at least with the individual's manager before formal sign-off, and experimental work.

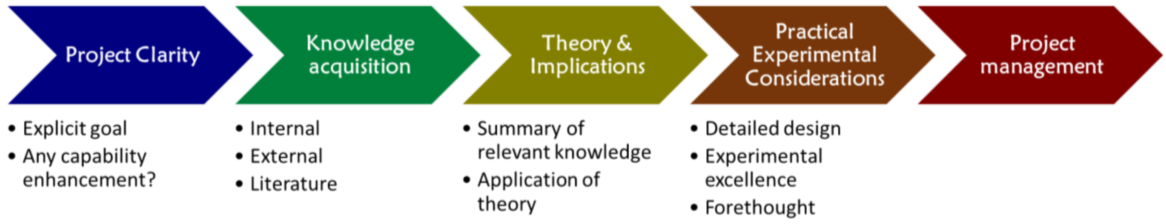

Figure 1. Successive steps in the ELN template.

3. Results and discussion

Actual experience, exemplified for mixing of a non-Newtonian fluid, showed that a compact document can be assembled with a moderate amount of effort. The compilation of relevant prior art and its implications enabled debate as well as the preparation of the later experimental work.

Strong managerial engagement to use and review the template during project discussions brought the approach alive. The best outcomes were obtained in "peer review"-type meetings. A mixed audience of both experimentalists and non-laboratory-based colleagues led to the best results. The ELN embedding allowed the framework to profit from the advantages thereof: sharability and formal validation steps; archival saving of additional insights and suggestions.

Some challenges in implementation also merit commentary. First, compiling and interpreting information takes time. Examples helped balance exhaustiveness and timeliness. Second, adoption was enhanced by writing the template steps in the natural order for performing the work.

The system has proven its value through use in many projects. By assisting scientific due diligence early on, it has ensured best long term use of resources. Specific examples include: pointing out the need for a more in-depth literature review; identifying additional measurements to be done; avoiding trials that were unlikely to lead to information; and emphasizing the calculations through which the information would ultimately be used.

Future opportunities include: the auto-generation of work reports; and modification for mathematical modeling. Different types of workflows, such as purely analytical work and academic exploratory work performed in the absence of theory, will also require adaptation.

4. Conclusions

A template has been devised to help systematize scientific work by clearly documenting: objectives; knowledge acquisition; relevant theory and its applications and expectations; and the resulting experimental considerations and plan. This framework, and its ELN implementation, enables systematic planning, as well as discussion and co-creation between researchers. The author invites others to adopt and adapt this new framework to systematize their own science workflows.

References

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