# Evaluation and Implementation of Biovia ELN software – Polymer group – DTU Chemical Eng.

**System:**

*System:* Biovia (Dassault Systèmes)

*Where is system used:* Polymer group, DTU Chemical Engineering

*What is the intended purpose of the system:*

* To secure documentation of experimental in research projects with students, including PhD students.
* Store relevant research information electronically instead of in written form.
* Ensure that the relevant experimental information is stored and saved for later use
* To avoid the transport of chemical traces out of the lab when taking the paper lab notebooks to the office

*How was the system chosen:*

The Biovia ELN was chosen by one of the PIs and group leader at the polymer group after taking part in one of the DTU ELN workshops. Different ELN software was presented by vendors and by DTU researchers during the workshop. The PI decided that Biovia would be the best option to test in his group. After a trial period of six months and a good evaluation from his group, they decided to continue with the use of Biovia as their documentation tool.

A more detailed description of the features required for an ELN system by this research group is presented in the Annex – Table 1.

**Users:**

*Number of users that the system is offered to and their backgrounds:*

Initially five licenses were purchased for the polymer group. After the six months of trial, other research teams in the same group were interested to test Biovia and five more licenses were purchased and distributed among those teams.

Today, there are 12-15 current clients which actively use the ELN. The number of experiments/entries is app. 530 in one and a half year.

**Organization:**

*What are the technical requirements of the system:*

For Web Users BIOVIA Notebook Cloud can be accessed by a browser based client where a native plugin must be installed to enable all functionality. It requires browsers that support this technology, such as Internet Explorer, Chrome, Firefox or Safari above certain versions specified in the System Requirements document provided by the vendor.

BIOVIA Notebook Cloud can also be accessed by the windows client, which can be downloaded via an administration tool provided by the vendor upon purchasing. Once the software is installed on a PC, the system will automatically download any new versions from the server.

*How is the technical installation and maintenance of the system organized:*

Data are stored on the Cloud services (located in the US) provided by Biovia. The data are automatically backed up daily by the vendor.

There is no local backup strategy until now. The PI coordinating this pilot project has backup the data on non-regular basis and once the department strategy in regards to ELNs is established, the department IT-support will be responsible to implement a backup strategy.

This group has detected what they consider a major disadvantage of the system in regards with backup that, experiments need to be submitted by the user before the administrator is able to download them. If students forget to submit their experiments, it is not possible to make a local backup of all the data.

*How is the administration of the system organized (e.g. maintenance of users, permissions, common content):*

The PI coordinating this pilot project has administered the accounts until now. In the future, it is expected to have a centralized administration of the ELN at the department, where the local IT- support should administer the ELN system including accounts management and the local backup of the data. Discussions in order to establish a strategy for documentation of experimental at a departmental level are taking place at the moment of the publication of this report.

Currently, there are no common templates to document the experiments. The structure of an experiment is up to the users. This is mainly because students do many different forms of experiments and as such it is difficult to have a common guideline.

The system has been organized by projects. Several students/users can submit their experiments and work actively in one project. This allows them to have an overview of all the data generated in that particular project and work collaboratively.

**Costs:**

*What are the license fees (if any):*

The 12 month purchase costs 100 Euros per year per seed (i.e. account)

*How are the running costs for system maintenance and administration financed (besides this activity):*

Running costs (also future licenses) will for now be covered by individual external grants.

Additional costs related to infrastructure has currently been solved by investments into a few things e.g. a label printer to be accessed by all users.

Computers for the labs are currently laid off laptops from former students. This is not ideal, but it seems to be working. In the long-term it is probably necessary to invest in a few new workstations for the lab.

**Overall experiences and future actions:**

The software is intuitive to use and everyone seems to have learned to use it really fast. Some things take bit longer to catch on i.e. copy / paste chemical structures seems to cause some problems in the beginning.

Biovia generally fulfills the group’s requirements. If you are doing standard work, it appears to work very well.

It takes a bit of time to adjust your workflows to the use of an ELN. For example, when working with multiple experiments in parallel with different type of samples. This would ordinarily also give problems with a paper lab notebook – and would normally have to be solved somehow from case to case. At the end, the user realizes that the ELN actually makes it easier to document also these many parallel experiments, as you can be a bit more systematic and copy/paste forms and information.

Mostly, data are written directly into the ELN. Only few notes are taken on paper (weighing compounds on the balance or similar). To some extent, some notes will have to be transferred, but this is dependent on the individual user.

The ELN real strength is in supervision and overview of projects as well as data backup. In addition, data can be read without bringing a lab book from the lab to an office which is a major advantage due to security reasons.

Some students who have been using the ELN extensively have stated that it definitely saves time on using this system rather than paper lab notebook.

Biovia can handle the file formats commonly used by the group i.e. asci or similar (native formats with limited file size) without problems.

The ELN search tool is very useful. Data are easily found.

Data sharing through the ELN system has been rather slow, but it is expected to increase. This is not related to the features of the ELN, but it is rather a question of the sharing culture of data at the department. Data sharing is more likely to happen in smaller groups where it is until now taking place and is working very well. The ELN has been very effective to share knowledge between students and supervisor, and also when students are part of bigger research projects.

On technical aspects, sometimes the system cannot be accessed or it is not possible to login to the administration of the profile. Logging in a little later usually solves the problem. However, a faster response of the server would be great.

The technical support offered by Biovia has always been fast and efficient.

Three main advantages of having the Biovia ELN:

* Overview of project for the PI
* Data sharing between users
* Controlling access to data between partners in a project.
* Repeated experimental systems and modularity during repetition.
* Safety in data storage and safety in preventing accidental transfer of compounds traces out of the labs.

Three disadvantages within the Biovia ELN.

* More specialized experiments are difficult to add into the lab book, where you for instance would like to combine drawing and sketching together with writing or handwritten notes of a setup. This takes longer time, and makes it a little less practical for exploratory research.
* It is difficult to upload data at locations where you cannot bring an electronic device, e.g. when you take notes close to the balance. This apply for our set up where we have PCs in the lab instead of iPads.
* Experiments have to be submitted in order to be downloadable. It is not possible to transfer the entire content of experiments to your own laptop or local storage system for backup. It has been a significant disadvantage. Alternatively, if users have left the group before submitting their experiments, you can email Biovia Support (BIOVIA.Support@3ds.com) and they can give you the rights to be able to change the author of an experiment, allowing you to then submit it yourself, which is not optimal.

# ANNEX – Requirements for an ELN system – Polymer group – DTU Chemical Eng.

## **Table 1. Relevant features for the selection of an ELN system Polymer group – DTU Chemical Eng**

