



E-Notebook for Productivity in Agrochemical Labs

Dow AgroSciences LLC, a subsidiary of the Dow AgroSciences Chemical

Company, discovers, develops, and brings to market crop protection and plant biotechnology solutions for the growing world. With a population projection of 9 billion by 2050, Dow AgroSciences innovates agrochemical and biotech solutions for increased crop productivity through higher yields, better varieties, and more targeted pest management. PerkinElmer's E-Notebook solution is the ELN of choice at Dow AgroSciences' R&D labs, predominantly in its North American sites, and also with users in Latin America and Asia Pacific locations.

Formulation Properties			
# of Units	Unit Mass Planned	Batch Mass Planned	Batch Mass Act.
1	7500	679.50 mg	6.60 kg
Batch Mass Act. 679.36 mg			

Step Name	Step Mass	Step Batch Mass	Mass Ratio	
1	Granulation	750 mg	15.00 g/g	
Materials				
Material	Role	Mass/Planned	Mass Act. / Mass	% of Total
1	AIJ212	12.47 % w/w	93.53 mg	10.63 %
2	Ethyl alcohol	36.57 % w/w	266.78 mg	30.33 %
3	Propylene glycol	11.33 % w/w	84.98 mg	9.66 %
4	Propylene glycol	2.00 % w/w	1.5 mg	1.71 %
5	Propylene glycol	17 % w/w	127.50 mg	14.93 %
6	Povidone	1.20 % w/w	9 mg	1.02 %

Name	% w/w Planned	% w/w Actual
1	AIJ212	0.74 %
2	Dimethicone	0.06 %
3	Eudragit 30% Phma	0.45 %

Figure 1: This screenshot shows a detailed formulation experiment set-up as part of the Formulations Module for E-Notebook.

An ELN Believer

Having relied on paper notebooks and the use of Microsoft® Office products, which still required cutting and pasting documents into the paper notebook, Dow AgroSciences in the mid-2000s was interested in the benefits of electronic laboratory notebooks for planning, capturing, recording, and analyzing scientific data. After a thorough evaluation of commercially available ELNs, the agricultural company selected and piloted E-Notebook in 2008 as a solution for:

- Productivity gains of 10-15 percent, based on implementations at other companies
- Improved data quality
- Intellectual Property protection
- Greater collaboration and access to accumulated data

E-Notebook, the most widely deployed ELN, is used by researchers in the chemical, food/flavor/fragrance, petrochemical, pharmaceutical, and biotech industries, as well as academic and government institutions. Its implementation at Dow AgroSciences is one of that industry's largest deployments.

Doug Brown, Dow AgroSciences' ELN project manager, said the company's strategy was to gradually roll E-Notebook out to chemists, biologists, and other R&D scientists, starting with a pilot team of 50. Lab groups eager to try an ELN were selected first, and all group members were required to test the E-Notebook to assess its impact on collaboration. Today, some 600 scientists use E-Notebook in Dow Agrosciences' R&D labs, where they are working on insecticides, herbicides, and fungicides, as well as fumigants, nitrogen stabilizers, and seeds, traits, and oils. In addition to creating and tracking individual group experiments and data, E-Notebook serves as a central data repository for long-term data archival for all R&D scientists to search, retrieve, and find the data that lead to the analyses that drive innovation.

Making Scientists' Jobs Easier

The screenshot displays a reaction section in the E-Notebook. At the top, there are chemical structures for the reactants and the product. Below the structures is a stoichiometry grid with columns for Run ID, Reactant, MW, PM, Limit, Eq, Sample Mass, Notes, Vol, Molarity, and % Wt. The grid contains three rows of reactants and one row for the product. Below the grid is a detailed procedure section with a 'Preparation' tab. The procedure text describes the reaction conditions, including the use of a magnetically stirred water/THF suspension, addition of (R)-2-amino-3-hydroxypropionic acid, sodium hydrogen carbonate, and benzyl carbonochloridate. The procedure also mentions the use of a dropping funnel and the addition of water. A 'Solvents' table is visible on the right side of the procedure section, listing Water and THF with their respective ratios and volumes. The interface also shows a 'Samples' table with columns for Selected, Sample ID, Exp #, Batch #, Temp ID, Source ID, Container ID, Amount, Units, Purity, Barcode, and Location.

Figure 2. The screenshot shows a reaction section in the E-Notebook. You can see that ChemDraw is embedded, the stoichiometry grid automatically pops up, and calculations are performed based on molecular weight and other factors.

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Doug Brown
Dow AgroSciences' ELN

A recent analysis of E-Notebook's strengths, weaknesses, opportunities, and threats by Dow AgroSciences lab leaders revealed the solution continues to “deliver on expectations” and help make the scientists' jobs easier. Scientists repeatedly list ease of data entry, importing/exporting files, and search and retrieve features as strengths that enhance productivity and collaboration. Broad use of templates allows users to standardize procedures and easily repeat or configure new experiments. Scientists also appreciate E-Notebook's standard integration with Microsoft Office products like Excel and Word, as well as numerous systems within the lab. Rather than entering data multiple times, E-Notebook can automatically share data with integrated systems.

In addition, PerkinElmer offers a number of add-on applications for compound registration, analysis request, inventory, multiproduct synthesis, formulations, supplemental data management, bioanalytical workflows, and more. Dow AgroSciences uses the inventory component of PerkinElmer's ChemBioOffice, its ChemACX chemical library, and formulation module for E-Notebook for formulation research. Dow AgroSciences is also evaluating use of additional bioanalytical workflow tools and enhancing our data analysis with integration of TIBCO Spotfire®. The ELN is additionally flexible through integration with third-party and homegrown systems. For example, Dow AgroSciences built integration to existing functionality from a third-party system for compound registration, rather than rip and replace it. Because it did not exist at the time the company deployed E-Notebook, Dow AgroSciences built a lab analysis request system to queue requests, send results to the requester, and store results in E-Notebook. This allows researchers from around the world, even in remote field stations, to interact with the system. “If we were to reevaluate that today, we might have come to a different decision,” Brown said, noting PerkinElmer has a commercial analysis request system available. “But six years ago, the best answer for us was to build that tool ourselves.”

The SWOT analysis also showed that data quality has improved first by eliminating the risk of transcription errors in manual processes, and also because users are far more likely to directly upload Excel spreadsheets and other supporting files to their experiments. This level of detail enriches the record, compared to summary notes that may have been written into a paper version. “You'd be more selective because handwriting information or gluing something into the paper notebook was more labor intensive,” Brown said. “Electronically, you can more easily add everything – spreadsheets with all the formulas. It helps you do things faster and you get better data.”

Brown says E-Notebook has helped with IP protection through the use of e-signatures, signing and witnessing functionality, and user access according to roles and responsibilities. Administrative functions enable lab managers to oversee activity and ensure that scientists are complying with corporate and other guidelines for protection of intellectual property. E-Notebook dashboards provide a good overview for managers on scientists' progress on experiments and sign/witness status, as well as other details. .

In terms of collaboration, the ELN earns high marks for making Dow AgroSciences' R&D data searchable and retrievable, as a long-term archive of experiments is maintained. As an essential technology that gets daily use, E-Notebook has proven to be reliable and fully functional. The increase in the number of scientists using E-Notebook has created a strong support network where people share best practices. After six years of use, Brown says E-Notebook is considered highly configurable, user friendly, and offers a broad range of functionality. "Sometimes it feels like we're only scratching the surface, of E-Notebook's capabilities" he says.

Dow AgroSciences keeps its eye on the ELN landscape. Describing PerkinElmer as "a true partner," Brown says PerkinElmer continues to develop its ELN and meet Dow AgroSciences' need. The companies have worked closely throughout the E-Notebook pilot of version 9, implementation of version 11, and upgrade to version 12, and Dow AgroSciences relies on PerkinElmer for ongoing technical support, custom workflows, and configuration assistance.

Next Steps

Brown says E-Notebook is now used by nearly every R&D scientist who requires notebook functionality, so future expansion will likely be from greater use of functionality. Already used for the management of chemical reference standards, E-Notebook will take on more Good Laboratory Practice (GLP) work by leveraging its signing and witnessing functionality. In addition, the administration features in E-Notebook allow lab managers to oversee scientists' work to help make better research decisions, discover hidden patterns, or identify batch effects within a screening. Brown says that the E-Notebook has become a daily way of life for Dow AgroScience scientists. Dow AgroSciences is very satisfied that they implemented the E-Notebook in 2008 because now they have eight years of electronic data that is date/time stamped, easily searchable and secures their intellectual property.

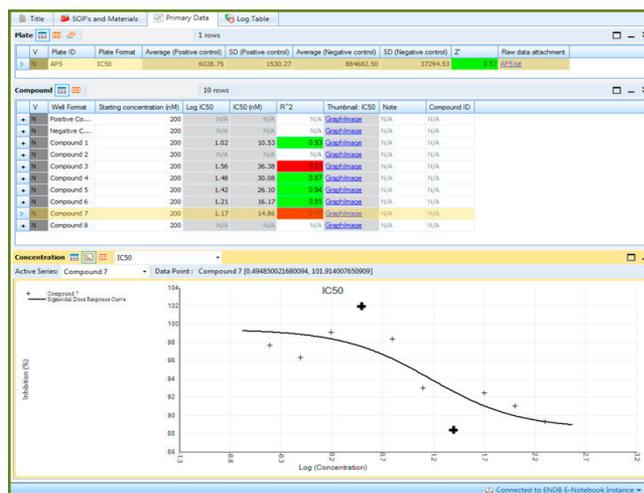


Figure 3. This is a screenshot of the Structured Data Module for E-Notebook, which is geared for biologists. Here you see an IC50 protocol with automatic curve fitting.