

OpenLAB Electronic Lab Notebook (ELN) for Synthetic Chemistry

Data Sheet

In an increasingly competitive environment, corporations must capitalize on scientific knowledge and discoveries faster and at reduced cost. You can compress project timelines by collaborating on projects and sharing knowledge to solve challenging synthesis problems. Agilent OpenLAB ELN helps you **design and document reactions much more efficiently**, share and reuse experimental protocols, and capture results directly from analytical instruments – all so you can **complete syntheses and receive analysis results in less time**. OpenLAB ELN enables you to:

- Search for reactions and compounds across in-house repositories or popular commercial sourcing and reaction databases
- Design new reactions and register products directly in your corporate compound registration system
- Create Dynamic Forms for routine procedures or commonly used phrases, for faster protocol creation
- Automate submission of samples for analyses, and access results the minute they are available

The screenshot displays the OpenLAB ELN interface for a synthesis protocol. At the top, it shows the project name 'M-NL-000006', the user 'Nicolas LOU', and the date '11-OCT-2009 17:54 CEST'. The protocol is for 'Antibiotics' and 'Cytosine'.

The reaction scheme shows the synthesis of a compound from two reactants. The reactants are 220.01 g/mol and 255.43 g/mol. The products are 233.39 g/mol and 175.23 g/mol. The reaction conditions are: 1. HCl, 13.00 PIPIC/A, PPH / Oh, 90 °C, 2. ethyl acetate.

The 'Solvents / Reagents' table is as follows:

Step	Solvents / Reagents	T	p
1	1.00 PIPIC/A, PPH / Oh, 90 °C	90 °C	bar
2	2.00 ethyl acetate	bc	bar

The 'Expected Results' table is as follows:

Structure	Additive	Formula	MW	Exp. Yield	Exp. Load	Exp. Qty.	Exp. Am.
		C ₁₃ H ₁₉ NO ₅ i	233.39	95.00		9.50 mmol	2.23 g
		C ₁₁ H ₁₃ NO	175.23	95.00		9.50 mmol	1.66 g

Figure 1. OpenLAB ELN interfaces with tools you already use, and helps you design syntheses more quickly and share knowledge across your organization.



OpenLAB ELN is a web-based open platform that increases your efficiency – while you use the tools and processes that already work in your organization. You plan and design reactions using the **tools you already know**, which **minimizes training** and **reduces ELN implementation time**.

- Design single and multi-step reactions with industry-standard tools from ChemAxon, Symyx, Accelrys, and CambridgeSoft
- Transfer reaction components to the materials section automatically and let OpenLAB ELN calculate the stoichiometry
- Create and manage multiple batches and easily split samples to request analyses

The flexible OpenLAB ELN integrates seamlessly with your existing registration systems and sourcing databases – to **speed discovery** and **protect intellectual property**.

- Access your company's compounds and transfer the associated data directly to and from OpenLAB ELN
- Find chemical building blocks and specialty compounds – without leaving OpenLAB ELN
- Drag and drop images and files directly into the experiment; add searchable annotations; and open files in the native application

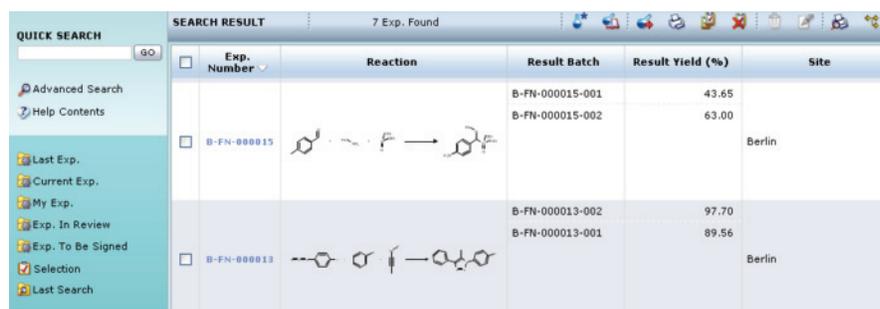
To learn more about
OpenLAB ELN, visit us at
www.agilent.com/chem/eln

OpenLAB ELN **removes the burden of repetitious “paperwork”** and gives you more time to focus on discoveries.

- Use Dynamic Forms to easily design standard templates and data entry forms, to capture experiment details rapidly and consistently
- Set up favorites for commonly used reagents and solvents, and quickly add them to your experiment
- Dynamically link to stoichiometry tables, to update your protocols automatically

OpenLAB ELN **increases collaboration** down the hall and across the world, **saving time and improving productivity**.

- Share information and reduce redundant experiments; search across molecules and reactions to find experiment details and results
- Use the Analytical Request Workflow to request and track analyses of your compounds, with immediate access to results



Exp. Number	Reaction	Result Batch	Result Yield (%)	Site
B-FN-000015		B-FN-000015-001 B-FN-000015-002	43.65 63.00	Berlin
B-FN-000013		B-FN-000013-002 B-FN-000013-001	97.70 89.56	Berlin

Figure 2. Search OpenLAB ELN to find similar reactions that have already been completed in your organization. Avoid duplication of results and make new discoveries faster

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Printed in the USA September 15, 2010
5990-5606EN



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