



At a Glance

We're helping to increase scientists' productivity by making it easy to capture data, archive it, share it, and protect intellectual property with our E-Notebook™ solution.

Enhance Scientists' Productivity in Your Organization

Developed in collaboration with scientists from many of the world's top R&D organizations, our E-Notebook solution for research and development provides a common workflow that embodies industry best practices for data capture, archiving, and intellectual property while creating a shareable archive to drive collaboration and innovation.

There are specialized capabilities for Chemistry, Biology, Formulations, and Analytical workflow management, making it the perfect enterprise-wide solution for your organization.

It's easy to see why researchers in the pharmaceutical, biotech, chemical, petrochemical,

food, and flavor and fragrance industries, as well as academic and government institutions, rely on E-Notebook to enhance personal productivity and improve data quality.

Capture, Store and Collaborate

Collaboration and innovation go together. Silos of data and information mean that valuable insights are either not shared or lost, resulting in wasted time and missed opportunities. With E-Notebook, storing and sharing insights and information such as experimental plans, chemical reaction schemes, and test results generated from the many experiments happening in your organization – today and in the future – is made easy. Many different formats are supported within E-Notebook including free text, tables, images, and graphs.

E-Notebook Highlights

- Provides a common workflow that supports industry best practices for data capture, archiving, and intellectual property

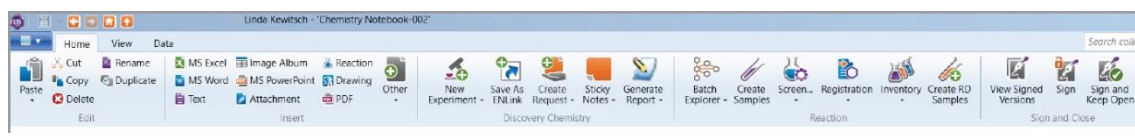


Figure 1. Ribbon menu control from an E-Notebook experiment.

- Creates a hub for information and data sharing that helps drive collaboration and innovation
- Allows requests for performing tests to be managed efficiently and effectively across your R&D organization
- Connects to other solutions for further productivity improvements and to gain greater value from your experimental data

Intelligent Data Capture: Data can be captured and stored easily from an extensive and diverse range of workflows, such as medicinal chemistry, biological assays, protein purification, fermentation, and formulation trials, enabling scientists to record all key information about their experiments.

Drag and Drop: To reduce the number of mouse clicks, the drag-and-drop feature lets users search and find files on their desktops or networks, then select and add files into their experiments. This automatically generates appropriate sections for each of the associated documents. Any files not recognized by E-Notebook are stored as an attachment. E-Notebook recognizes Microsoft® Office files, including Word® documents, Excel® spreadsheets, and PowerPoint® presentations, PDFs, ASCIIs, and image files. The drag-and-drop feature extends to moving experiments around within E-Notebook folders, copying an experiment or experiment sections between notebooks and rearranging sections or tabs in an experiment.

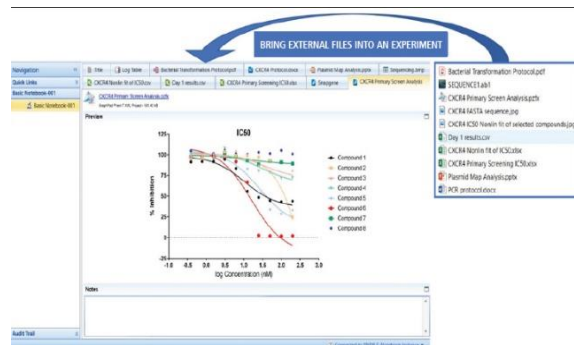


Figure 2. Drag-and-drop files from your computer to add files to an experiment in E-Notebook.

Time-saving Tables: Get to interesting data quickly through effective sorting, grouping, and filtering

using tables. Settings are saved with the experiment for future use, and images are easily moved and stored within tables.

Integration with Microsoft® Office: There is a tight integration with Microsoft® Office (Word®, Excel® and PowerPoint®). External editing provides all the functionality of Microsoft® while maintaining the user experience. With external editing, users can select which part of the document to display as a preview.

Search and Find: Search and retrieval from records – even across experiments – is made easy, allowing knowledge sharing and reuse of information across project teams and your organization. You can search text across all types of E-Notebook records using Boolean queries, domain selection, and other advanced options, as well as chemical structures and reactions.

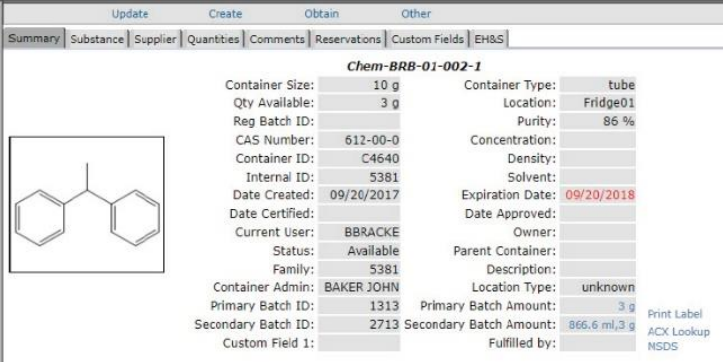
Organize Data and Teams: Configure the different levels of organization to fit your business needs. Add sites, business units, departments, user groups, and projects to organize your E-Notebook and experiments.

Equipment Management: Track, manage routine upkeep, and store important documentation within E-Notebook using the Equipment Management functionality. Equipment used in experiments are automatically linked and tracked through metadata and log files, alerting scientists to calibration, specification or expiration dates.

Equipment Type	Reference	Vendor	Model	Serial #	Status	Calibration Expiration	Service Type
1 Biosensor	WPA6 Biosensor System 200840 102 Analog	GE Healthcare Life Science		080001	0801	25-Apr-2019 10:49:22 AM -0500	Calibration
2 Pipette	Class 150	Class	P 18	#02742	1547	23-Aug-2019 12:42:19 PM -0500	PM
3 Pipette	Class 1500	Class	P300	#9822245	1587	24-Oct-2019 12:06:08 PM -0500	Calibration
4 pH Meter	751 Minus Station 1	Kovach	4712 34	132323	3394	18-Aug-2019 10:12:21 AM -0500	Calibration
5 Pipette	1500A Pipette	Thermo Scientific	N/A	30080611	3719	18-Aug-2019 10:12:21 AM -0500	Calibration
6 Balance	Delta Balance	Carver/duPont	Test Model	TCE3	3751	23-Oct-2019 10:39:52 PM -0500	Verification

Figure 3. Equipment, Materials, Solutions and Stockroom can be managed with E-Notebook's Equipment Management capabilities.

Tracking: Add registration integration to track registered substances and batches, including custom metadata and business logic to support specific business requirements such as property calculations and alternative duplicate checking. Use the inventory solution to track inventory including substances, structures, containers, plates, locations, racks and freezers, all in a single system.



The screenshot displays a software interface for tracking substances. On the left, there is a chemical structure of 1-phenylethylbenzene. To its right is a table of metadata for the substance, identified as Chem-BRB-01-002-1. The table includes fields for container size, availability, registration batch ID, CAS number, container ID, internal ID, creation and certification dates, current user, status, family, container administrator, primary and secondary batch IDs, container type, location, purity, concentration, density, solvent, expiration and approval dates, owner, parent container, description, location type, primary and secondary batch amounts, and fulfillment status. A 'Print Label' button is visible at the bottom right of the table.

Chem-BRB-01-002-1			
Container Size:	10 g	Container Type:	tube
Qty Available:	3 g	Location:	Fridge01
Reg Batch ID:		Purity:	86 %
CAS Number:	612-00-0	Concentration:	
Container ID:	C4640	Density:	
Internal ID:	5381	Solvent:	
Date Created:	09/20/2017	Expiration Date:	09/20/2018
Date Certified:		Date Approved:	
Current User:	BBRACKE	Owner:	
Status:	Available	Parent Container:	
Family:	5381	Description:	
Container Admin:	BAKER JOHN	Location Type:	unknown
Primary Batch ID:	1313	Primary Batch Amount:	3 g
Secondary Batch ID:	2713	Secondary Batch Amount:	866.6 ml, 3 g
Custom Field 1:		Fulfilled by:	

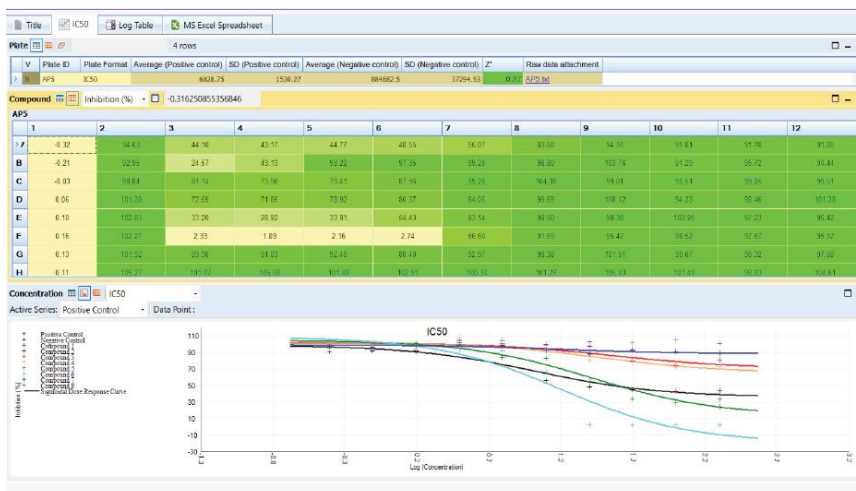
Figure 4. Clicking on the barcode in E-Notebook allows you to view the container holding the material in inventory.

Supplementary Data Management: For laboratories with multiple instruments and users, the SDM module enables immediate, automatic access of all instrument output files, images and PDFs within the E-Notebook experiments. Users can reference, import, or export most file types at their convenience. An enhanced version provides centralized management of multiple files with automatic import from multiple users.

Accelerate Biological Workflows:

A range of specialized features for managing biological assay data - including ready-to-go protocols for a range of common assays and tools to design, edit, and sort protocols and workflows - help make designing and running assays faster and easier, so biologists can spend more time on biology.

The image to the right represents IC50 Protocol comparing curves for three compounds selected from a plate.



Enhanced Productivity for Chemists:

Integration with our ChemDraw® chemical intelligence software, with ChemACX, Inventory and Registration are just a few ways that E-Notebook provides advanced capabilities for chemists to help them to work more efficiently.

The image to the right represents a sample screen of a dynamically created stoichiometry table.

Reagent	Product	Limit?	MF	FM	%w	d	Eq	Sample Mass	Moles	Mol.	Vol	Barcode	Updated
1 I	3-HYDROXYACETOPHENONE	<input type="checkbox"/>	C ₈ H ₈ O ₂	136...			1.000	0.737 g	5.41 mmol			152	<input checked="" type="checkbox"/>
2 II	3-bromo-5-methyl-1,5-dihydro-2H-pyrido[3,2-b]pyridin-2-ylidene	<input checked="" type="checkbox"/>	C ₁₄ H ₁₀ N ₂ C	277...			1.000	1.5 g	5.41 mmol				<input type="checkbox"/>
3 III	DMS	<input type="checkbox"/>	C ₂ H ₆ S	62.1...	0.84...		1.000	0.336 g	5.41 mmol		0.400 ml		<input type="checkbox"/>
4 IV	dicyanozinc	<input type="checkbox"/>	C ₂ N ₂ Zn	117...			1.000	0.636 g	5.41 mmol				<input type="checkbox"/>
1 V	P1		5-methyl-2-oxo-2,5-dihydro-1H-pyrido[3,2-b]pyridin-2-ylidene	C ₁₄ H ₁₀ N ₂ O	223.2...		1.206 g	1 g	96.6 %	82 %	5.41 ml...		4.42 mmol

Faster Formulations Development:

Effectively document and exploit knowledge gained from experiments using E-Notebook's specialized tools for formulation scientists, including predefined and user-definable calculations and materials, and a multistep formulation summary that allows users to drill down into the underlying formulation to record information.

The image to the right represents a sample screen for planning of a formulation. Materials can be added in multisteps and all calculations are dynamic.

Step Name	Step Mass	Step Vol	Mass Ratio	Vol Ratio	% w/w of Total
Mixing Step	1000 mg		100.00 %		100.00 % w/w

Material ID	Material	Role	Mass	Density	Batch Mass	Mass/Mass	Act. Mass	Act. Mass/Mass	% Mass of Total	Mass Delta
1	Ranitidine	API	336 mg		336.00 mg	33.60 % w/w	333 mg	33.43 % w/w	33.60 %	1.00 mg
2	Citric acid	Stabilizer	128.0 mg		128.00 mg	12.80 % w/w	127.9 mg	12.76 % w/w	12.80 %	900.00 µg
3	Na bicarbonate	Preservative	146.1 mg		146.10 mg	14.61 % w/w	146.1 mg	14.58 % w/w	14.61 %	0.00 mg
4	Mannitol	Sweetener	150 mg		150.00 mg	15.00 % w/w	150 mg	14.97 % w/w	15.00 %	0.00 mg
5	Sorbitol	pH	100 mg		100.00 mg	10.00 % w/w	100 mg	9.98 % w/w	10.00 %	0.00 mg
6	Aspartame	Sweetener	80 mg		80.00 mg	8.00 % w/w	80 mg	7.98 % w/w	8.00 %	0.00 mg
7	Sucrose	Coating	20 mg		20.00 mg	2.00 % w/w	20 mg	2.00 % w/w	2.00 %	0.00 mg

In combination with Active Directory, it will tag file imports with the user ID for simpler file selection.

Make: With E-Notebook you can more effectively plan, perform, and document experiments to avoid duplication of work and to maximize knowledge gained from experiments.

- Plan, execute, and record experiments and create a secure searchable archive of intellectual property
- Automatically name compounds, calculate stoichiometry, and achieve rapid input of experimental methods
- Accurately draw, store, search, retrieve, publish, and display structures and reactions with the capabilities of our industry-leading ChemDraw software
- Efficiently create and share chemically intelligent, publication-ready structures and use the structures to generate names, explore 3D shapes, calculate properties, and predict spectra
- Search for compounds and data with a variety of tools to facilitate structure-property correlation and decision making
- Drill down into the underlying formulation to record information, including analytical data per formulation using the multistep formulation summary capability
- Group experiments, explore the data using powerful data pivot tools with integrated graphing, isolate critical variables easily using drag and drop, and visualize relationships with the formulation aggregation tools
- Check the novelty of compounds and mixtures and assign unique identifiers to enable data linking and integration

Test: Create, submit, and manage requests to perform tests across your R&D organization efficiently and effectively with E-Notebook.

- Select from a set of preloaded service/request types or custom-configured service/request types
- Submit a sample with a request to have it analyzed by the corresponding department
- Keep track of your samples, see who has them, and locate where they're stored
- Report structured and unstructured results back to requestor
- Keep track of requests and tasks based on your role using dashboards, which provide information sets such as request and tasks ID, status, stakeholders, and links to collections related to a request (samples, test, experiments)

Components	Structure	MP	MPN	Peak Mass	Theor. Mol. Weight	Actual Mol. Weight	Purity	Yield
1,2-dimethyl-5-methyl-7-(3-methylbut-3-en-2-yl)-1H-imidazo[4,5-b]pyridine	<chem>CN1C=NC2=C(N1)C(C)C=C(C)C2</chem>	CarbAlu20	264.220	1.405 g	5.32 mmol	1.3 g	43.0 mmol	91 %

Properties

Amount: 1 mg
 Barcode: A1101
 Source of Sample: Chem 888-02-012
 Project: Catalyst Synthesis
 Project Number:
 Lot #

Reaction

1,2-dimethyl-5-methyl-7-(3-methylbut-3-en-2-yl)-1H-imidazo[4,5-b]pyridine + H₂O → 1,2-dimethyl-5-methyl-7-(3-methylbut-3-en-2-yl)-1H-imidazo[4,5-b]pyridine-3-ol

Test Results

Sample ID	Sample ID	Request ID	Task Log	Comment	Status	Purity	Yield	Integration
1-100112	Chem 888-02-012	Request 000170	Request 000170	Request 000170	Complete	91 %	91 %	Complete

Figure 5. Samples keep track of all the work done on them during their life cycle, providing a one-stop source of information

Decide: Query, search, and analyze data to help you make decisions using Structured Data Management.

This highly flexible method of capturing data allows it to be queried and searched more easily.

By defining a series of fields, calculations and curve fit models, E-Notebook constructs a single table or series of hierarchical tables that store and process raw data from an experiment or test. Once the section is built, it becomes part of the experiment. E-Notebook then automatically loads, calculates, and displays all the data and results. A comprehensive mapping wizard helps users map their data formats, visually and interactively, using templates that can be reused for multiple experiments.

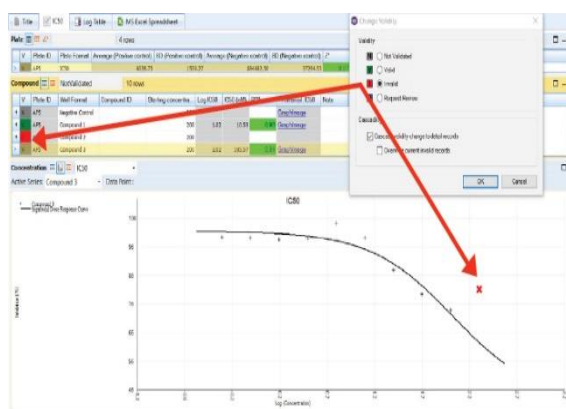


Figure 6. Data validation in the structured data management tool.

In addition, you can link E-Notebook and Spotfire® visualization and analysis software to uncover new insights from your R&D data and make better, more informed decisions. Data is easily uploaded to Spotfire® so that you can carry out advanced analysis across multiple or individual experiments, identify relationships, isolate outliers, and spot patterns. Spotfire® analysis file (.dxp) templates can be dragged back into E-Notebook for safe storage with the related experiments. Users can also open the file to review the analysis when new data becomes available.

Connect: By connecting E-Notebook to other solutions you can further improve productivity and unleash even greater value from your experimental data.

Connecting to Registration provides a highly configurable and flexible registration system for chemical and mixture registration. This enables users to track registered substances and batches of those substances, add custom metadata, business logic, and add-ins to support specific business requirements such as property calculations and alternative duplicate checking, and assigned configurable unique identifiers to registered substances and batches.

You can also integrate with the Inventory capabilities for additional functionality. This allows the tracking of substances, structures, containers, plates, locations, racks, and freezers so that you can easily manage the availability, whereabouts, and quantities of substances – either in a single stockroom or across multiple sites. It also means scientists can find out what is available, where it is located, and how to safely handle, store and dispose of materials.

Start Saving Time Today

It's time to make your organization and its scientists more productive by introducing E-Notebook – the ideal user-friendly solution for capturing, archiving, and sharing data and protecting intellectual property. With this powerful and intuitive tool, you can drive enhanced collaboration, innovation, and productivity across your organization.

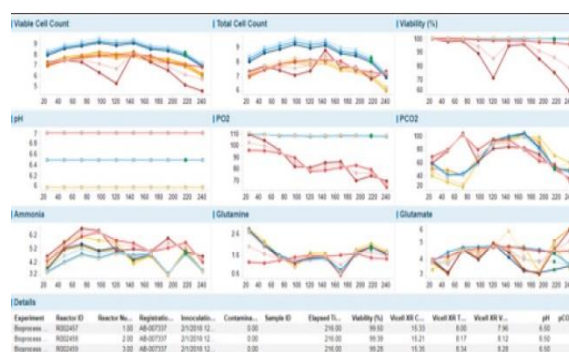


Figure 7: Snapshot of data and experiment parameters within a single frame from E-Notebook presented in Spotfire from a representative fermentation process within a biologicals environment.