

## An Enterprise Electronic Lab Notebook: Designed by Scientists



**“Global enterprises and CRO's are calling for a single enterprise notebook that can be used worldwide across business ventures. Such an ELN should enable multiple project teams and scientific disciplines to access, analyse, and share experimental data over global networks.”**

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To be successful, electronic lab notebooks (ELNs) must meet the day-to-day needs of the scientists who use it. This is especially critical for enterprise ELNs designed for use across scientific disciplines.

Symyx Notebook is the result of the company's broad experience developing ELNs for large, global corporations over the course of 15 years. Close collaboration with numerous pharmaceutical companies has been essential in understanding the workflows and use cases encountered by scientists in their daily activities.

“The key really is asking scientists what they actually need and then partnering to build that core functionality into the system correctly right from the beginning, rather than giving scientists what you think they want and then hoping for good results,” said Stan Piper, Senior Scientist, at Pfizer Inc, which was one of seven companies that has partnered with Symyx on the development of its Notebook. “It's a long haul process that requires constant feedback over many iterations.”

Essential to success, according to Piper, is choosing a vendor that “agrees on your vision of the product—which is not always as easy as it would seem—and who has the capacity to partner with a large organisation effectively to build an out-of-the-box, fully supported solution. For us, Symyx was that partner.”

### IMPROVED DATA QUALITY

During critical paper prototyping some scientists at Pfizer requested more flexible ways to capture and record experimental data. Version 6.1 lets scientists enter data manually, using the notebook's auto-fill capability, or capturing data directly from lab equipment for improved consistency. Configurable tables enable biologists to capture animal species, body weights, dates, doses, and responses. Analytical

chemists can record equipment, reagents, and samples including names, molecular weights, total volumes, concentrations, etc. The tables also offer integrated calculations and customisable data views (e.g. the ability to filter, group, and sort data items). With searchable tabular data, a scientist can quickly find specific information, such as all documents that reference ‘Balance 384’ or ‘Acetonitrile Lot 1223.’

Integration with nearly all modern Mettler-Toledo and Sartorius balances enables scientists to record actual amounts directly from balances.

Daily balance checks and up-to-date calibration information in the context of an experiment can be accessed. Notebook 6.1 is extensible via a full software developer kit that supports client-server integration and custom development.

Extension points include integration with statistical analysis, kinetic modeling, and PK/PD modeling software as well as a variety of instruments and database systems including LIMS for sample management and data repositories such as the Waters NuGenesis SDMS. Integration with the company's own Assay Explorer biology data management system or Plate Manager software can also speed the collection, analysis, and reporting of biological results (Figure 1).

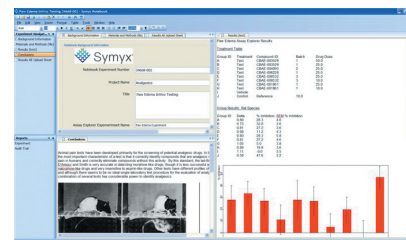


Figure 1. Symyx Notebook 6.1 lets biologists load reports from a biology data management system; capture observations in real time as they record results; annotate and summarise results; and make decisions based on all parameters (whether recorded, processed, or observed).

## ENHANCED COLLABORATION

The Notebook enables multiple project teams and scientific disciplines to access, analyse, and share experimental data over global networks, a requirement becoming increasingly critical with the volumes of work out-sourced to third-party contract research organisations in India, China, and other locations.

Another collaborative functionality for analytical chemists and biologists is the ability to insert "sticky notes" into an experiment, which encourages collaborative dialogue between authors and reviewers.

In response to customer feedback, these comments are not stored as part of the versioned document and can be deleted at any time.

Experiment referencing (via hyperlink) also improves experimentation and

collaboration by enabling chemists and biologists to trace the reuse of materials from one experiment to the next and quickly determine which of their experiments have been referenced in colleagues' work (Figure 2).

The screenshot shows two tables from the Symyx Notebook 6.1 interface. The top table is titled 'Reagents' and lists various reagents with columns for Name, Source, Lot #, Rate, Expiry Date, Comments, and Referenced. The bottom table is titled 'References' and lists references with columns for Reference, Type, Description, Applied to, Last Modified by, and Last Modified On.

Name	Source	Lot #	Rate	Expiry Date	Comments	Referenced
1 Acetonitrile	Sigma-Aldrich	143283	Solvent	31/12/2009	MP.C. grade	Y
2 Tetrahydrofuran	Thermo Scientific	JB28103	Reagent	31/12/2009		Y
3 Deionized water	In house		Solvent	31/12/2009		Y
4 100% DMSO/A	Preparation		Mobile Phase	12/26/2008	Mobile Phase A	Y
5.1						Y

Reference	Type	Description	Applied to	Last Modified by	Last Modified On
1	Reagent	Acetonitrile from Reagent	Prep	MSHALL@PMPH.com	12/22/09 1:46:25 PM
2	Reagent	Tetrahydrofuran from Reagent	Prep	MSHALL@PMPH.com	12/22/09 1:46:25 PM
3	Reagent	Deionized water from Reagent	Prep	MSHALL@PMPH.com	12/22/09 1:46:25 PM

Figure 2. Symyx Notebook 6.1 lets scientists reference multiple experiments directly in the notebook (via hyperlink), making it easy to trace the use of materials from one experiment to another and determine which experiments have been referenced by colleagues.

## CONCLUSIONS

Symyx Notebook has been designed to be the hub of a scientist's workday, the place where scientists orchestrate the design, execution, analysis, and reporting of experiments. It is designed to be used out-of-the-box across multiple scientific disciplines including analytical chemistry, synthesis, and biology, from discovery through manufacturing. Built on a robust, scalable, and secure informatics platform, Symyx Notebook consolidates experimental data, forms data, and text into fully versioned, searchable documents that can be shared over global networks with project team members and contract research organisations. Symyx Notebook is the result of close collaboration with several large pharmaceutical companies and broad experience with discipline-specific notebooks in large, multi-site deployments.

## Multivariate Data Analysis Software Update

Umetrics has announced the release of a 64-bit edition of its multivariate data analysis software SIMCA-P+ (currently in version 12.01) designed to accommodate very large data sets.

SIMCA-P+ 64 version 12.01 with a suitable 64-bit processor, and the 64-bit version of the MS-Windows operating system Vista, allows the analysis of large data sets well beyond the 2 GB limits of RAM available for the 32-bit version.

64-bit versions of the on-line modules of the SIMCA suite, SIMCA-Batch On-Line, SIMCA-4000, and Q (for embedding) will follow soon.

The SIMCA-P+ 12.01 software is 21 CFR part 11 compliant for immediate use in the pharmaceutical and biotech industries, from R&D to manufacturing.

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## Expanded Capabilities for Greater Flexibility in Image Analysis

GE Healthcare announces the launch of IN Cell Investigator v1.5 software, the latest addition to the Investigator range of user-friendly image analysis tools for automated high content analysis of live and fixed cells. The new features of the software provide users with the highest flexibility, meeting the needs of a wide range of image analysis activities in sub-cellular research and screening. In addition to building on over 50 validated applications, the new features of IN Cell Investigator v1.5 facilitate: whole well analysis - the generation of a panoramic image through image stitching of overlapping images enables the analysis of whole wells, larger cell populations and model organisms; texture analysis - for deeper insight into results, particularly for toxicology and cell cycle; 3D-angiogenic tubules formation analysis; de-clumping of heavily clustered colonies and populations containing binucleated cells, providing greater insight into stem cell colony analysis; and cell feature tracking to get a temporal perspective of cellular processes.

In conjunction with the IN Cell Miner software, Investigator v1.5 offers a fully integrated solution for image analysis, data management and visualisation that can be used with all IN Cell Analyser systems from GE Healthcare, including the recently launched IN Cell Analyser 2000. Additional options of the software facilitate the integration of high-content data from the IN Cell Analyser with other third-party sources. High quality technical support is available for IN Cell Investigator v1.5, including onsite training courses and customised training based on individual requirements.

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