

## CONNECTING INFORMATION ACROSS THE LAB

### THE CHALLENGE

#### REMOVING OBSTACLES TO DATA SHARING AND RESEARCH DECISION MAKING

Scientists, particularly those working in a GxP environment, rely on laboratory information management systems (LIMS) to centralize and manage data across projects and studies. A LIMS can handle even the most complex study protocols and interface directly with instrumentation, all while tracking experimental details, collecting data, and providing audit trails to satisfy regulatory requirements. Yet in many cases, scientists still record individual experimental details and observations in paper notebooks. In addition to creating data transcription errors and referencing issues, this disconnect between electronic systems and paper notebooks prevents scientists from rapidly locating critical historical information on their colleagues' work—unless they enjoy thumbing through scores of archived paper notebooks.

### THE SOLUTION

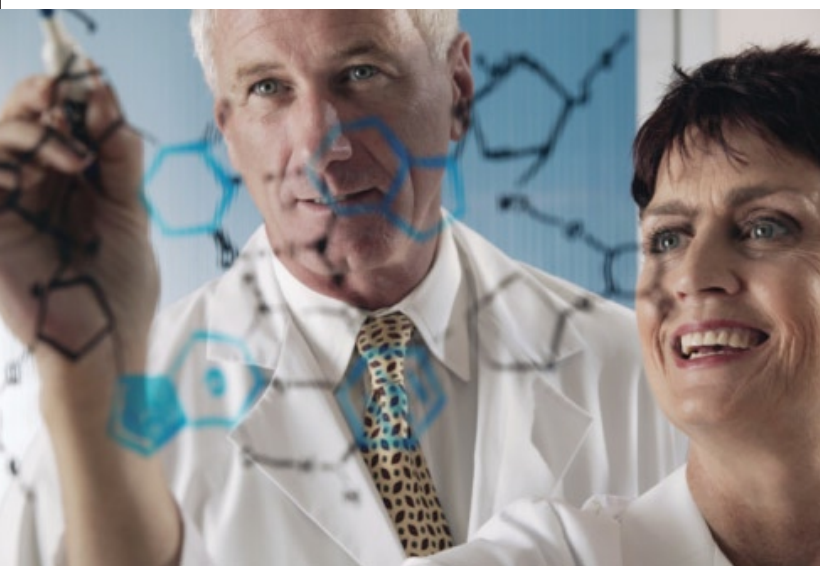
#### INTEGRATION BETWEEN THERMO SCIENTIFIC WATSON LIMS AND SYMYX NOTEBOOK

The first development in the recently announced partnership between Thermo Fisher Scientific and Symyx (see article, p. 4) is integration between Thermo Scientific Watson LIMS and Symyx Notebook enterprise electronic laboratory notebook (ELN). The integration enables scientists to:

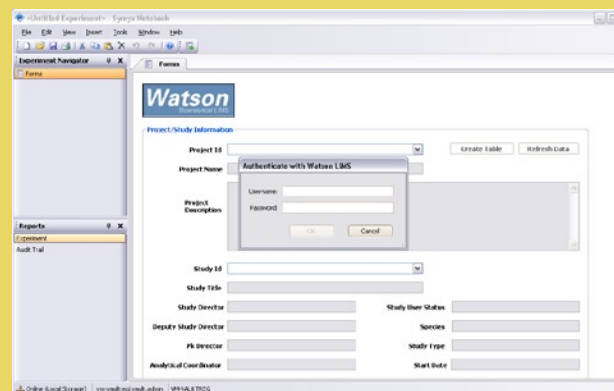
- Design studies in Watson LIMS
- Transfer sample information from Symyx Notebook into Watson LIMS
- Document lab activities (including sample preparation) in Symyx Notebook
- Generate Watson LIMS worklists that can also be annotated in Symyx Notebook
- Transfer completed Watson LIMS reports back to Symyx Notebook.

Symyx Notebook, as well, is fully GLP compliant, so that every step of the process or addition to a study is securely tracked and referenced.

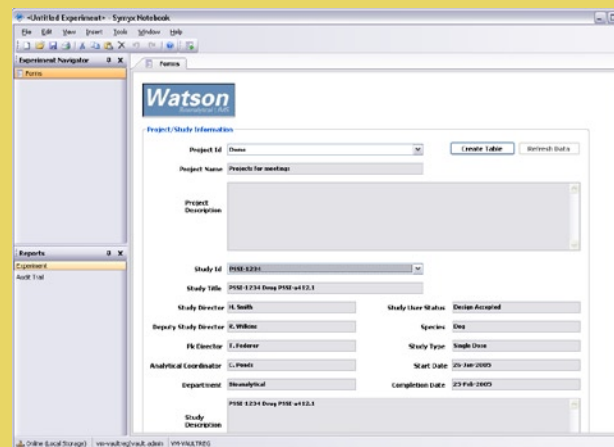
One advantage of the integration between Watson LIMS and Symyx Notebook is that scientists can work within the system they prefer. For instance, scientists who have entered sample information in Symyx Notebook can extract other experimental details from Watson LIMS by entering their login credentials (see next page). Similarly, as will be pointed out later, scientists using Watson LIMS can make similar connections to Symyx Notebook to share reports with colleagues or clone experimental protocols. The integration ensures that all experimental details on projects or studies are authenticated by the LIMS and documented electronically.



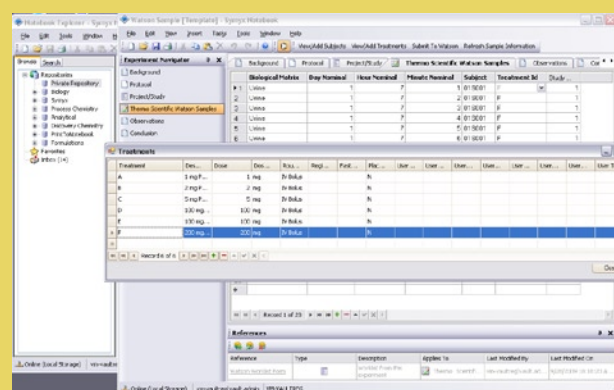
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Having established the connection to Watson LIMS, scientists simply enter a project and study ID (privileges can be set to ensure that scientists can only access projects on which they are working). Watson LIMS then automatically populates the read-only fields in Symyx Notebook with the appropriate, authenticated study details (below).

The integrated systems also greatly simplify sample handling between Symyx Notebook and Watson LIMS. In this case, scientists use dropdown menus to select specific study details, such as biological matrix, subject, and treatment information. Watson LIMS automatically populates each sample form with the appropriate information. The screen below shows a collection of urine samples, all taken for subject 01S001 (screen not shown), who received treatment F. Crucially, information is easy to update as studies progress over time; additional details added in the notebook can then be updated in Watson LIMS, and all project, study, and sample information is searchable using standard Symyx Notebook functionality.

Once the study protocol has been accepted, scientists generate Watson LIMS worklists, clean-up the samples and add any necessary annotations to Symyx Notebook and then analyze the samples on the laboratory instruments. Watson LIMS sends instruments the appropriate files to create a sequence, but only after sample preparation has been completed. In most labs, this step is still documented by technicians using paper processes. The integration between Symyx Notebook and Watson LIMS enables any scientist (not just the one who created the study) to log in to Symyx Notebook, select the project and study, and import a worklist (a complete list of study samples, quality controls, and standards to prepare and run on the instrument) to Watson LIMS.

## JAMES JACK



James Jack is currently a senior consultant in ELN application services at Symyx. He joined MDL Information Systems as a customer support representative in 1999 after receiving his Ph.D. from the University of Aberdeen in organometallic chemistry. Three years later, he became a member of MDL's consulting group and has since worked on many high-profile customer projects and some of Symyx's most innovative products, most recently the popular ChemMobi iPhone app.

### HOW DOES SOMEONE WITH A PH.D. IN ORGANOMETALLIC CHEMISTRY END UP A TOP-NOTCH SOFTWARE DEVELOPER?

My Ph.D. work was at the interface between organometallics and vibrational spectroscopy. Studying the activation of the particular compounds we were interested in required some computation work, namely 3 by 3 force constant refinements and a Fortran 77 program called ASYM20. ASYM20 could handle 20 atoms, and one of my tasks was to turn ASYM20 into ASYM40. This experience, along with a general interest in programming (at the time Visual Basic 1.0), led me to take on some "freelance" development work for the chemistry department. I developed systems to

help enroll undergraduates, manage timetables, and store and report students' laboratory marks. By the time I finished my Ph.D., I was pretty sure I wanted to work in the area of cheminformatics, and I got the chance to do so when I was hired by MDL.

### IN YOUR TEN YEARS WORKING WITH CUSTOMERS AND DEVELOPING CHEMINFORMATICS SYSTEMS, WHAT CHANGES HAVE HAD THE BIGGEST IMPACT ON YOUR WORK?

It's amazing how much computing has progressed in the last 10 years. Megabytes have become gigabytes, and Moore's law keeps plodding on, leading to more powerful devices capable of running much more demanding software. And where there is a need for really heavy processing, web services have come along to make that easy too. All of this means that we developers can build truly intuitive software. Applications I have been working on recently—Structure Resolver, Chemistry Desktop, ChemMobi—all make use of the power that today's computing technology brings, embedding web services and performing non-intrusive tasks for scientists without them even having to ask.

### WHICH PROJECT IN YOUR CAREER WAS MOST REWARDING TO WORK ON AND WHY?

While all of the many projects I've worked on have been interesting in one way or another, I have to say that the applications I work on in my spare hours have been the most rewarding to create. I enjoy

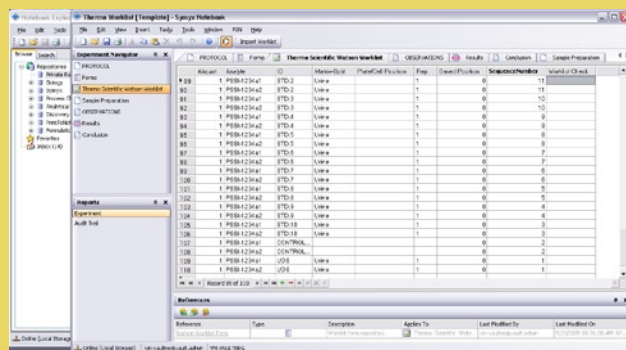
developing all the cool add-ins for Symyx Draw and hope they highlight what a great drawing package we have. I have recently turned my hand to developing add-ins for Symyx Notebook, and again the speed with which you can develop powerful extensions tells me that we have a good architecture under the hood.

"YOU NEVER KNOW WHEN INSPIRATION WILL STRIKE! THE MOST IMPORTANT THING FOR ME IS TO LISTEN AND TO READ BETWEEN THE LINES TO BUILD UP A FULL PICTURE OF WHAT THE SOLUTION NEEDS TO DO."

### WHAT'S YOUR "TYPICAL" APPROACH TO CONSULTING PROJECTS?

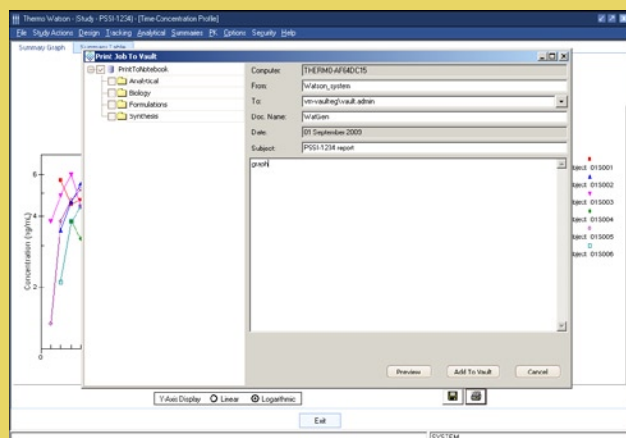
I have some of my best ideas when I least expect them: in the shower or waiting for my wife in a supermarket car park are good examples. You never know when inspiration will strike! The most important thing for me is to listen and to read between the lines to build up a full picture of what the solution needs to do. Often customers will shy away from issues that they envisage as being technically difficult to achieve, but which are needed to deliver a complete solution. It's a consultant's job to show them that in fact the full vision is achievable and to deliver it on schedule and within estimate.

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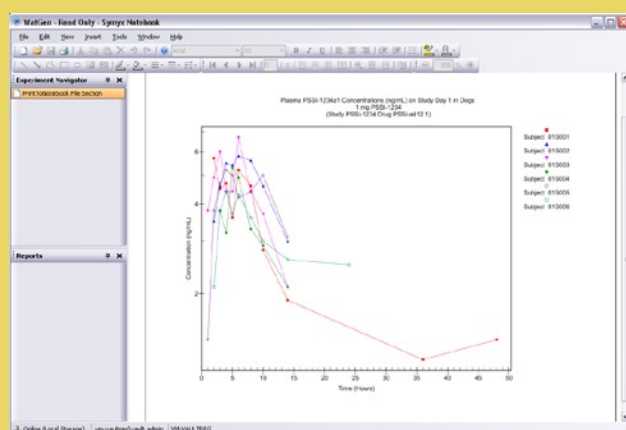
Data is collected and processed by Watson LIMS, and reports can be easily exported back to Symyx Notebook. The first screen below shows in the background a Watson LIMS concentration-versus-time profile for several subjects.

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Scientists can use the Print Job to Vault option to export a read-only version of the graph to Symyx Notebook (below).

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In addition to the integration described here, Symyx and Thermo Fisher Scientific have used ISENTIS to enable scientists using Watson LIMS to connect to Symyx's extensive collection of biotransformation content in databases like Metabolite (see the Spring 2009 issue of Molecular Connection). Contact Symyx to find out how to use Symyx Notebook, ISENTIS, and Watson LIMS to better integrate your laboratory. For more information about Thermo Scientific Watson LIMS, visit [www.thermo.com/watson](http://www.thermo.com/watson).