

Benchware Notebook

Scientific Planning, Documentation and Collaboration



Based on the requirements of laboratory scientists, Benchware® Notebook supports research operations at large, multisite organizations as well as small, single-site companies. In addition to enhancing end user workflows, Benchware Notebook provides an open, service-oriented architecture that is designed to cost-effectively integrate with existing enterprise systems, including Laboratory Information Management Systems (LIMS), compound registration and inventory tracking systems. Furthermore, Benchware Notebook enables creation of a searchable record of research activity, giving research management an easy view into the experimental history, and simplifying the process of bringing together information required to file and defend patent applications.

Key Benefits

Laboratory Scientists:

- Improves scientific planning and eliminates duplication of past experiments
- Facilitates quick and easy data capture through autocalculation cut-and-paste, and page cloning functionality

Research Management:

- Enhances current research through the creation of a broadly accessible, enterprise-wide scientific knowledge base
- Improves the efficiency of the research operation by reducing paperwork and enforcing standardized and legible data capture

Legal/ Patent Professionals:

- Implements company IP capture processes and creates a database of research activity easily accessible to legal teams for rapid investigation on patent and FDA compliance issues

IT Professionals:

- Facilitates cost-effective integration with legacy and 3rd party informatics systems through the use of standard web-services technologies, a fully documented API, and an included Software Developers Kit (SDK).

Improve Workflows to Increase Research Efficiency

Developed in collaboration with practicing laboratory scientists, Benchware Notebook was designed to reduce paperwork and repetitive tasks. In addition, with all pertinent information available at one's fingertips, report generation is simplified, no longer requiring manual searching for and reproduction of archived material. Auto-calculation functionality within a Benchware Notebook page allows scientists to easily determine important experimental factors.

Support Diverse Operations

Each notebook page is a collection of components, which represent specific types of data or pieces of a workflow. Customized page components can also be defined and added by a system administrator, and can be created to be domain-specific to disciplines such as medicinal chemistry, parallel chemistry, high throughput chemistry, genomics, screening, ADME and toxicology.

Support the IP Process

Benchware Notebook offers full tracking of page history and revisions and automatically captures dates in support of "first to invent" patent claims. In addition, the context for this information is built into the system, providing a clear means of tracing records, events, and dates to support patent claims.

Search and Learn from Past Research Efforts

Benchware Notebook's fast search system allows arbitrarily complex queries to be quickly built and executed by end users. With all entered data stored in an underlying Oracle® database, Benchware Notebook users are able to dynamically search within their own notebook pages and pages of others across the organization. Searches can

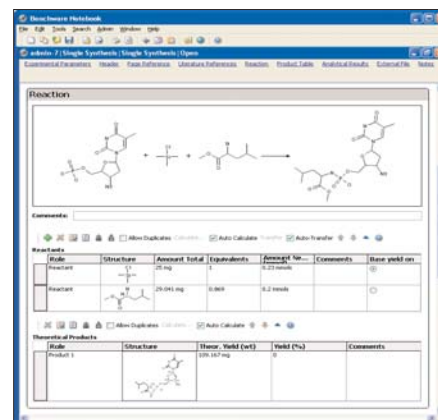
be done by using conventional alphanumeric search terms as well as by using more complex 'discipline-centric' search terms.

Designed for Enterprise Integration

Benchware Notebook was designed to allow a variety of systems to be easily tied together into seamless workflows for scientists, while at the same time providing a flexible integration framework.

Michael Elliott, president of Atrium Research & Consulting, a leading market research firm focused on the growing ELN market, says:

"The discovery informatics market is moving away from standalone applications toward integrated solution suites to improve program team collaboration and innovation. Benchware Notebook will help to accelerate the movement from monolithic ELNs to open and modular collaborative environments that address the needs of the end users while protecting valuable intellectual property."



Example of Benchware Notebook being used to record a chemical synthesis experiment. Reactions are imported, reagent amounts entered, and yields automatically calculated in Benchware Notebook.

Complementary Offerings:

Benchware LibraryMaker

Benchware LibraryMaker is an intuitive application for enumerating both small parallel libraries as well as very large virtual combinatorial libraries.

SMART-IDEA

SMART-IDEA allows researchers and corporate decision makers to have on-demand access to disparate types of research information on which to base pivotal drug discovery decisions.

Benchware Notebook uses truly open technologies, versus proprietary web-service protocols, to create a set of well-defined application program interfaces (APIs) and web services. Using the included Software Development Kit, informatics teams can quickly connect Benchware Notebook to other existing enterprise systems and/or desktop tools, and modify these connections over time to meet changing business needs.

Laboratory Page Creation

- Support many types of discipline-specific pages with minimal configuration
- Clone existing pages to create new, similar pages
- Record relationships to other pages or literature references
- Attach and view files within a page
- Create revision history for changes and annotations to pages
- Out-of-the-box Chemistry Module includes the following functionality:
 - Draw new reactions in standard sketcher programs such as MDL® ISIS/Draw and ChemDraw®
 - Import reactions and structures from 3rd party files such as MOL, SD, RXN
 - Automatically calculate structural information from the reaction
 - Automatically calculate reactant requirements based upon equivalents
 - Automatically convert between weight and volume for samples
 - Attach and show analytical information, including spectra

Integration

- Integrate with existing systems using an open API based on web-services

Advanced Searching

- Explorer-like interface organizes your personal pages into any nested hierarchy for easy retrieval
- Search reaction components by exact match, substructure, and similarity
- Retrieve a page by its name through one-step searching
- Flexibly search through an advanced query builder
- Flexibly view results
- Enter an unlimited number of keywords for easy searches to your pages
- Search reagent lists
- Export results to text files and MS Excel

Security

- Manage access to pages and all associated information through database-level access control
- Set business rules to allow or deny access to individual notebook pages
- Configure detailed security rules to prevent or allow access to individual features

Administration

- Create new page templates, and associate with existing sections
- Configure existing formats to require information
- Create page templates for each customized workflow, and guarantee adherence to corporate standards
- Dynamically update lookup lists, projects, users, etc
- Easily manage user security and configuration

Benchware Notebook Case Study
Schering AG:

Benchware Notebook is currently being used by over 400 users at three Schering AG sites worldwide and provides support for planning and synthesis of drug-like compounds. In this environment, Benchware Notebook was integrated directly to several legacy systems, including compound registration systems and systems for analytical data capture.

Dr. Rolf Jautelet, Medical Chemist at Schering AG says:

"Benchware Notebook greatly enhances the way experiments are planned, captured, managed and shared at Schering AG. Using this innovative tool makes it very easy for me to collaborate with colleagues all over the world and to draw inspiration from the collective scientific works of the organization."

Installation Recommendations
Server System

- Windows® Server
- Oracle 10g
- 2 GHz+ Intel or compatible processor
- 2 GB RAM

Client System

- Windows XP Professional
- 1 GHz+ Intel or compatible processor
- 256 MB RAM (minimum)
512 MB RAM (recommended)
- ISIS/Draw 2.4 (or later)
- ChemDraw 9.0.2



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