

Benchware

Laboratory Informatics Software for Discovery Chemists



Benchware® is a unique suite of laboratory informatics software specifically designed to meet the challenging demands placed on today's discovery chemists.

By combining powerful and proven discovery software with the experience and intuition chemists use every day, Benchware helps discovery scientists capture and share valuable insights with their colleagues, while providing them with the autonomy to confidently make better decisions about which compounds to synthesize, acquire, or test next.

Key Benefits

Laboratory Chemists:

- Provides laboratory chemists with the autonomy to make better decisions about which compounds to synthesize, acquire, or test next
- Increases productivity by accelerating decision making ability in the laboratory
- Easy and quick utilization of the models, procedures, and results produced and validated by expert computational chemists
- Enhances communication and workflow between laboratory chemists and other research groups

Computational Chemists:

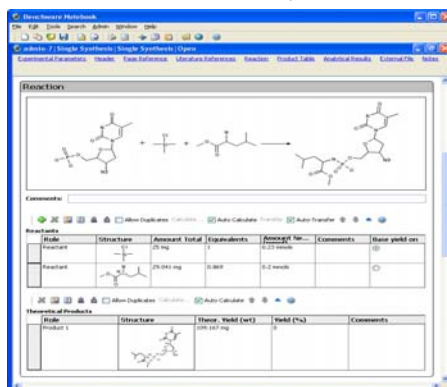
- Improved management of modeling knowledge through centralized capture of models, procedures, and results
- Enhanced Return on Investment in modeling infrastructure through improved utilization and visibility of modeling results
- Reduces workload of computational chemists, allowing them to focus time on non-routine tasks best handled by expert users
- Time saved on performing routine calculations

Discover Benchware

Benchware products spark innovation, accelerate decision making, and enhance collaboration by supplying laboratory chemists with data, information, and knowledge produced by specialists within the chemistry organization and other research departments. Armed with new information, laboratory chemists use Benchware products to plan experiments, increase productivity, and conduct real-time predictive studies in areas such as ligand-receptor interaction and small parallel library design. Built with the entire organization in mind, Benchware products make it easy for researchers to understand their data, rapidly design and conduct experiments, and communicate findings to the discovery team. Benchware products include:

Benchware Notebook

Developed in collaboration with practicing chemists at Schering AG and Tripos Discovery Research, Benchware Notebook is designed to be the accepted place to plan, conduct, document, and share drug discovery research. Rather than storing information in disparate archives, scientists can enter their plans, results,

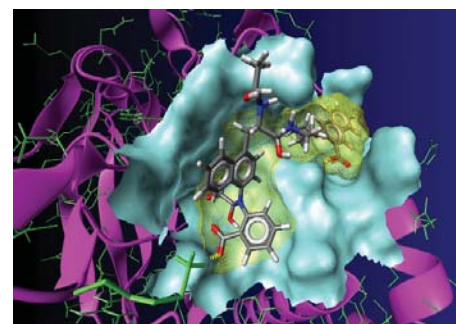


Reactions are imported, reagent amounts entered, and yields automatically calculated in Benchware Notebook.

observations, analyses, and conclusions through a single interface to create an integrated, searchable knowledgebase.

Benchware 3D Explorer

Benchware 3D Explorer's state-of-the-art molecular graphics, user-friendly interface, and communication capabilities allow researchers to view, share, and understand complex molecular data and 3D chemical information. Benchware 3D Explorer has been designed explicitly to allow communication of molecular models, procedures, and results between laboratory scientists and their colleagues in computational chemistry. By utilizing an open development environment, IT specialists may integrate the application with other tools and workflows within the organization. Benchware 3D Explorer was formerly marketed as LITHIUM.



PDB structure 1NNY displayed in Benchware 3D Explorer depicts a potent, selective protein tyrosine phosphatase 1B inhibitor. Strong, selective binding of the ligand is achieved through hydrogen bonding (yellow dashed lines) and shape complementarity between the ligand and the protein binding site is shown by the juxtaposition of their Connolly surfaces.

Complementary Offerings:

SYBYL®

SYBYL's completely integrated environment for computational chemistry and molecular modeling provides the fundamental components for understanding molecular structure and properties with a special focus on the creation of new chemical entities.

Tripos Professional Services

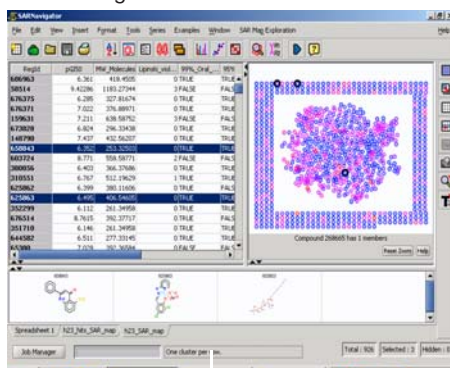
The Tripos Professional Services team is available to customize and integrate Benchware products into existing enterprise systems and workflows, ensuring that a total solution is provided to meet specific business needs.

Benchware Dock

Benchware Dock allows laboratory chemists to test compound ideas in real time against a 3D model of the target protein structure using docking procedures created and validated by expert molecular modelers. With Benchware Dock, chemists can now perform iterative design cycles for lead compound modification, docking, and review in minutes instead of days or weeks while allowing modelers to concentrate on the development of enhanced predictive models.

Benchware HTS DataMiner

Benchware HTS DataMiner offers a breadth and depth of functionality dedicated to the location, definition, and prioritization of prospective lead series from screening data sets of any size. Through two state-of-the-art chemical data mining techniques, SAR Maps and SAR Rules, and a host of chemistry-oriented data analysis capabilities, Benchware HTS DataMiner provides users with the validated science and workflow support needed for modern HTS and vHTS data analysis. Benchware HTS DataMiner was formerly marketed as SARNavigator.™



Datasets can be explored in Benchware HTS DataMiner using spreadsheet, scatter plots, histograms, correlation coefficients, and advanced visualization such as similarity maps and bull's-eye plots for high-throughput screening data analysis.

Benchware LibraryMaker

Benchware LibraryMaker is an intuitive application for enumerating both small parallel libraries as well as very large virtual combinatorial libraries. Benchware LibraryMaker was designed to provide both computational and laboratory chemists with an easy-to-use interface and to provide the features most relevant to today's industrial drug and molecular discovery challenges.

Benchware LibraryDesigner

To make both small parallel and large combinatorial compound libraries, chemists must decide which reactants to use, usually from a very long list of potential reactants. Benchware LibraryDesigner was developed to assist the laboratory chemist specifically with this decision-making process.

New Products to Come

Development is currently underway on new Benchware applications to be launched in late 2005 and early 2006. New applications will take advantage of Tripos' Service Oriented Informatics framework and will aid chemists in areas such as Molecular Alignment and Structure Activity Relationship (SAR) analysis.

Benchware Case Studies

Schering AG:

Benchware Notebook was born during Tripos' collaboration with Schering AG to build an enterprise chemical informatics system. The system built and deployed was specifically designed to store the drug discovery company's chemical registration, inventory, and ordering data and provide support for planning, synthesis and logistics of all compounds.

Built on the same electronic laboratory notebook platform available to Tripos customers as Benchware Notebook, the Tripos developed solution allows Schering scientists to efficiently manage research plans; access chemical information from across the organization; and immediately determine what materials are on hand to use in their research.

Apath, LLC:

Apath, an early-stage drug discovery company based in St. Louis, MO, is focused on the development of broad-spectrum antiviral agents for RNA viruses, which today are poorly treatable or entirely untreatable with currently available medications.

Using the Benchware HTS DataMiner desktop analysis tool granted to Apath as part of Tripos' Hits-to-Leads program, Apath has been able to attack a problem prevalent throughout the drug discovery industry: finding and defining the chemical series that have the BEST chances of moving into pre-clinical.