Benchware Discovery 360°

Integrated Data Access, Analysis, and Decision Support

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Benchware® Discovery 360° is a ground-breaking Integrated Discovery Environment that provides scientists and research managers with a single point of entry from which they can access, analyze & share data from disparate repositories of biological and chemical data. Group workspaces and powerful analysis tools within Benchware Discovery 360° make it easy for users to share and make sense of complex research data, leading to streamlined project team collaboration and better informed decisions.

Key Benefits

Research Management:

- Enables better informed decisions to be made based on complete and actionable research information
- Facilitates collaboration and communication between project team members and departments
- Greatly reduces the amount of time scientific teams spend on retrieving, manipulating, analyzing, and distributing data
- Eliminates redundant experimentation, leading to direct cost savings

IT Management:

- Reduces IT time and overheard spent on tactical data retrieval requests
- Use of true W3C SOAP technologies leads to cost-effective system integration, maintainance and support

Laboratory Scientists:

- Allows use of multiple best-of-breed data analysis tools in one application
- More time spent on scientific innovation, less time on data retrieval and management
- Automates manual and tedious data transformation tasks

The Problem: Current Methods of Data Access and Analysis

In today's complex drug discovery landscape, project teams base decisions on data pulled together from numerous experiments and databases. Trends are typically extracted from these data using the dozens of domain-specific analysis applications available to the researcher at the time.

Unfortunately, there are often obstacles between scientists and the data they require. Data generated by other groups may be stored in a local "silo" accessible only through the intervention of an IT person or key data may be in a format incompatible with analysis tools, and require the assistance of someone with specialized scripting skills.

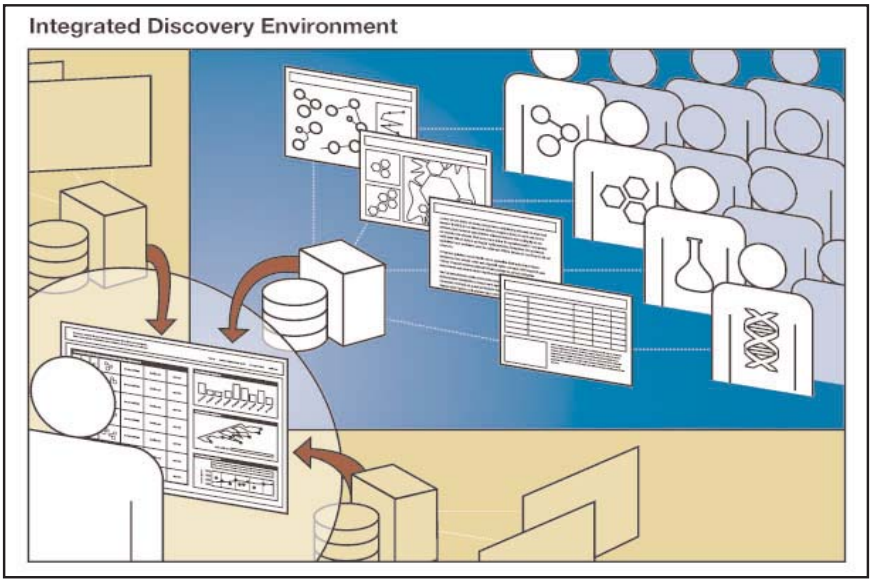
These hurdles may be individually surmountable, but taken together, across multiple project teams within one discovery organization; they lead to many person-years of wasted effort.

The Solution: An Integrated Discovery Environment

In an effort to overcome these obstacles and increase productivity, pharmaceutical firms are seeking to implement integrated, cross-disciplinary, and holistic approaches to making research decisions.

In order to bring these approaches to life, it is imperative that pharmaceutical organizations be able to implement an enterprise-wide infrastructure that catalyzes strategic decision-making and streamlines information distribution across all stages of the drug lifecycle.

Tripos developed Benchware Discovery 360°, the first commercially available Integrated Discovery Environment, to help drug discovery organizations enable such approaches. Benchware Discovery 360° allows organizations to gain better insight into their own drug discovery projects, improve scientific collaboration, and allow project teams to fully realize the value in the data they are generating.



Above: Benchware Discovery 360° is an Integrated Discovery Environment that allows users to access and analyze, through a single point of entry, corporate repositories of structural, biological, and chemical data.

Complementary Enterprise Offerings

Benchware 3D Explorer

Benchware 3D Explorer offers a configurable environment that allows non-computational researchers to view and interact with complex 3D molecular information at the desktop. The application facilitates communication between drug discovery team members by allowing them to easily create and exchange 3D models.

Benchware Notebook

Benchware Notebook is Tripos' enterprise electronic laboratory notebook (ELN) application, already in use by hundreds of scientists around the world. Designed in collaboration with scientists at multiple drug discovery sites to be a true 'Enterprise-Class' ELN, Benchware Notebook is set apart by its open, plug-in based integration framework and intuitive user interface.

A Powerful Components-Based Offering

The Benchware Discovery 360° offering is comprised of the following components:

D360° Client Application

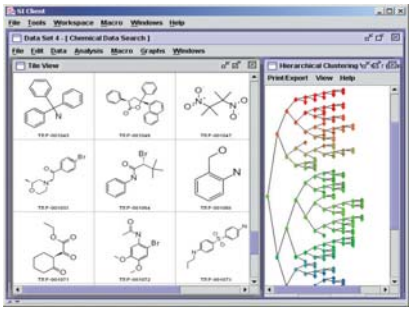
- This client application serves as the user's interface to the Benchware Discovery 360° system and allows users to intuitively input queries, view results, analyze data, and participate in group workflows. The D360° Client includes:
  - Standard Spreadsheet and Graphing Tools
  - Integration Points for Third-Party Visualization and Analysis Tools
  - Graphical Access to Private and Public Workspaces
  - Macro Functionality for Automating Commonly Used Workflows and Creating Dynamic Data Views
  - Integrated On-Line Help System

FormsBuilder Client Application

- This Drag-and-drop user interface allows researchers to dynamically build custom querying forms. Self-serve access to forms reduces reliance on IT, allows scientists to focus on science and allows IT personnel to focus on more strategic tasks.
  - Create, Save, and Share New Templates in D360° workspaces

D360° Server

- This standards-based (Apache Tomcat, JBoss, Apache Axis) application server, provides for:
  - Workspace Management
  - Job Management
  - Session Management
  - Communication with Tripos Integration Engine



Benchware Discovery 360° is used to visualize and select interesting compounds from a database.

D360° Workspaces

- These modules allow scientists to share results and analyses at project, Therapeutic Area (TA), and global levels. Workspaces allow project team members to communicate and share information and best practices as if they were all in the same geographic location.

Tripos Integration Engine

- Based on award-winning Enterprise Information Integration (EII) technology from Composite Software, the Tripos Integration Engine recognizes and treats multiple data sources as one virtual database. Creating a virtual database removes the necessity of the user having to know anything about the format and location of stored data. The Tripos Integration Engine also:
  - Generates and Optimizes Queries and Server results
  - Provides for On-the-Fly Data Manipulation

Tripos Compute Engine Framework

- The Tripos Compute Engine Framework allows access to Tripos and 3rd party compute engines, allowing users to use the powerful property calculators and compute engines that they may already be familiar with.

Case Study: Bristol-Myers Squibb

The Benchware Discovery 360° offering grew out of Tripos' relationship with Bristol-Myers Squibb (BMS). Bristol-Myers Squibb needed to streamline their drug discovery processes to reduce time-to-market and costs.

To address these concerns, Tripos partnered with BMS to create and deploy the SMART-IDEA application. SMART-IDEA is used at BMS as a workspace environment where chemists and biologists consolidate and analyze structural, biological, and chemical data.

SMART-IDEA allows both scientists and managers within BMS to pull up essential project information when they need it, and in a format that suits their needs.

The current Benchware Discovery 360° offering is based on SMART-IDEA technology, and is scheduled to be deployed by Wyeth Pharmaceuticals later this year as part of its 'Next-Generation Discovery IT' initiative.

The Following Best-of-Breed Tools Are Compatible with with Benchware Discovery 360°:

- Spotfire® Decision-Site
- CambridgeSoft ChemDraw®
- MDL® ISIS/Draw
- Microsoft® Excel

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Benchware 3D Explorer

3D Chemical Visualization and Decision Support

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Benchware® 3D Explorer empowers laboratory scientists to make more effective research decisions by allowing them to visualize, annotate, share and experiment with 3D chemical structural information and the results of computational research. State-of-the-art molecular graphics, user-friendly interfaces, and communication capabilities allow researchers to view, share, and understand complex molecular data such as protein-ligand crystal structures, docking results, molecular alignments, or other 3D chemical information. Finally, standard VBA scripting capabilities within Benchware 3D Explorer provide the ability to customize and distribute task-based interfaces and applications based on specific organizational research needs.

Key Benefits
Laboratory Chemists:

- Provides highest quality molecular visualization capabilities on a Windows PC platform allowing researchers that are not expert molecular modelers to gain access to vital research information.
- Benchware 3D Explorer's intuitive 3D editor allows new chemical ideas to be created and explored in the context of supporting data prior to actual synthesis.
- Macro recording capabilities allow repetitive tasks to be automated. Macro scripts can be shared throughout an organization to ensure consistency of research operations.
- Provides connected knowledge capture capability through hyperlinkable captions.
- Supports scientist workflows through integration with key productivity applications.

Computational Chemists:

- Provides a mechanism for modeling groups to readily share their models and results with chemistry and biology researchers, improving ROI on modeling resources and better supporting chemistry and biology operations.

IT Professionals:

- Provides a platform for rapid development and deployment of custom cheminformatics solutions and applications. Custom-developed solutions take advantage of proprietary knowledge and increase the efficiency and effectiveness of end user research.

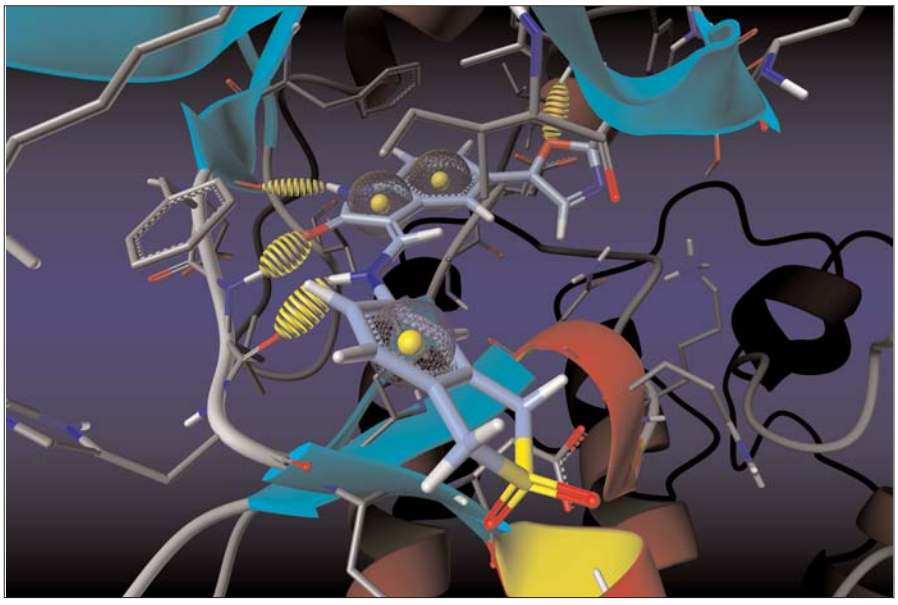
3D Molecular Visualization

Benchware 3D Explorer supports all standard visualization formats for molecular structure including solvent accessible and interaction surface computations with property mapping. Visualization of biological macromolecules is enhanced by the addition of protein and DNA/RNA ribbons. Both inter- and intra-molecular interactions such as hydrogen bonding and interatomic bumps can also be visualized, as well as prospective hydrogen-bonding regions. With the ability to render pharmacophores and 3D queries, Benchware 3D Explorer is a valuable tool for visualizing 3D information over all types of discovery projects.

For situations where a full 3D view of data is vital, Benchware 3D Explorer supports stereo viewing for both side-by-side methods and hardware.

Contextual 3D Molecular Editing

Benchware 3D Explorer's contextual 3D molecular editor allows any researcher to examine new candidate molecules within their biological context. The 3D molecular editor is modeled on widely used 2D sketchers familiar to life sciences researchers. Most importantly, the molecular editor allows the creation and modification of molecular structures in the context of a protein facilitating the exploration of new molecules within the constraints of target biological systems. The editor allows researchers to rapidly prototype new molecular structures.



PDB structure 1KE7 displayed in Benchware 3D Explorer depicts a potent, Oxindole-based CDK2 inhibitor. Hydrogen bonding interactions between the ligand an protein backbone and sidechains are depicted by yellow dashed ovoids whose width denotes the strength of the hydrogen bond. Key hydrophobic pharmacophore sites in the ligand are denoted my meshed spheres.

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.

Benchware® Discovery 360

The Benchware Discovery 360 data access, analysis and collaboration system addresses research productivity issues by combining a single point of access to all discovery data with a connected data analysis environment and workspaces that allow researchers to easily share their findings.

Communication and Knowledge Management

Benchware 3D Explorer users can share their insights and knowledge with other researchers by adding viewpoints, annotation, and hyperlinkable captions to 3D molecular structure data. Sessions can be saved and shared through email and shared file systems, or Benchware 3D Explorer can be used as a web browser helper application.

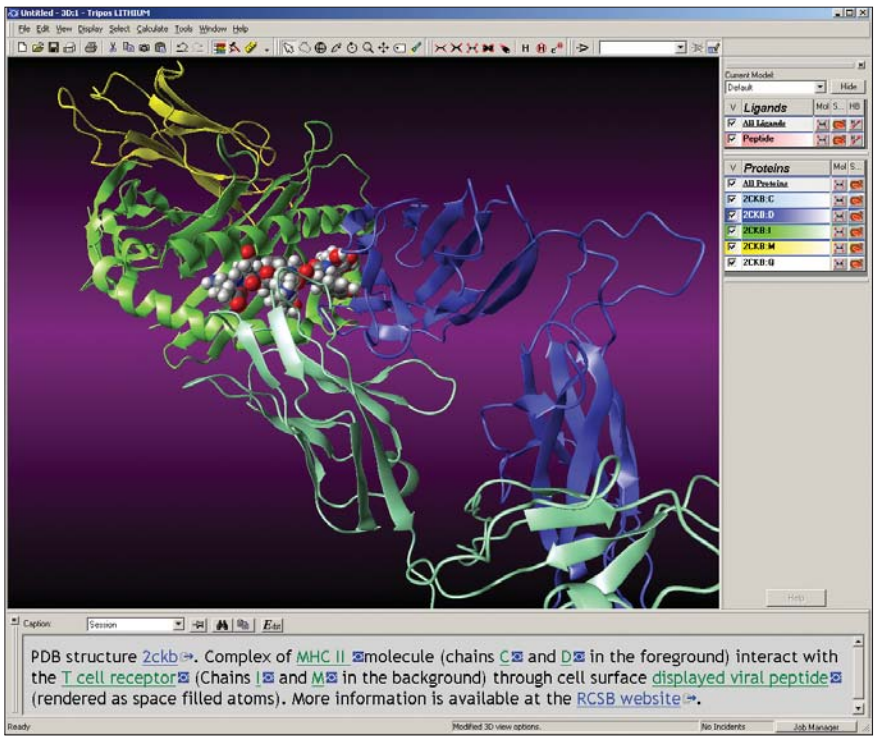
Cut and paste between Benchware 3D Explorer and OLE-compliant Windows productivity applications (Word®, Excel®, PowerPoint®, and Outlook®) and chemistry sketching packages (ChemDraw™ and MDL® ISIS/Draw) provides a standard mechanism for users to present their findings and data in presentations and reports while maintaining access to the original data.

Integration with Powerpoint allows users to incorporate live 3D views into their presentations for truly interactive communication of 3D chemical information.

Benchware 3D Explorer contains macro recording and playback capabilities allowing users to automate repetitive tasks and share useful macros with colleagues. Benchware 3D Explorer also has the ability to run VBA scripts created using developer features.

Development and Delivery with Benchware 3D Explorer

The full power of Benchware 3D Explorer is available through industry-standard VBA scripting. All functionality, from manipulation of molecular structure to control of graphical objects, and creation of task-based graphical user interfaces can be achieved through the application's VBA interface. Benchware 3D Explorer contains spreadsheet, graphing, and web browser components that can be accessed and customized through VBA to develop task-specific applications. Using the built-in browser component, chemistry web applications can be directly delivered through Benchware 3D Explorer's chemically intelligent interface. This allows organizations to integrate web services into chemistry applications, rather than creating chemistry applications from a web browser.



Benchware 3D Explorer's viewpoints and associated captioning capability allow users to associate their knowledge and insights to structural data presented in Benchware 3D Explorer. Caption text can be hyperlinked to any selectable object in Benchware 3D Explorer such as molecules, atoms, surfaces, and molecular interactions; as well as external files and web pages. Benchware 3D Explorer's captions allow straightforward knowledge capture and navigation by subsequent viewers, thereby extracting maximum value from structural information.

Visualization

- Import and export a wide variety of chemical structure and related file formats (mol2, sdf, MDL mol, SMILES, PDB, etc.)
- Visualize pharamacophores and 3D molecular queries
- Atom mapping and configurable ligand extraction upon reading PDB files
- Tight integration with Chemdraw and Cut and Paste structures from standard chemistry sketching packages (Chemdraw, MDL ISIS Draw)
- State-of-the-art OpenGL graphics
- Standard molecular rendering styles (lines, capped sticks, ball & stick, space fill, tapered bonds)
- Compute and display molecular surfaces (Connolly and Lee & Richards) and protein ribbons.
- Property mapping onto surfaces and ribbons
- Electron density and Isosurface display for whole molecules and spatial regions (from standard electron density files and gridded molecular field data).
- Inter- and intra-molecular interaction display (bumps and hydrogen bonds)
- Comprehensive atom selection tools
- Hardware and side-by-side stereo-in-a-window 3D viewing capability
- Advanced display manager with ability to select structures, generate sub-groups, and create models

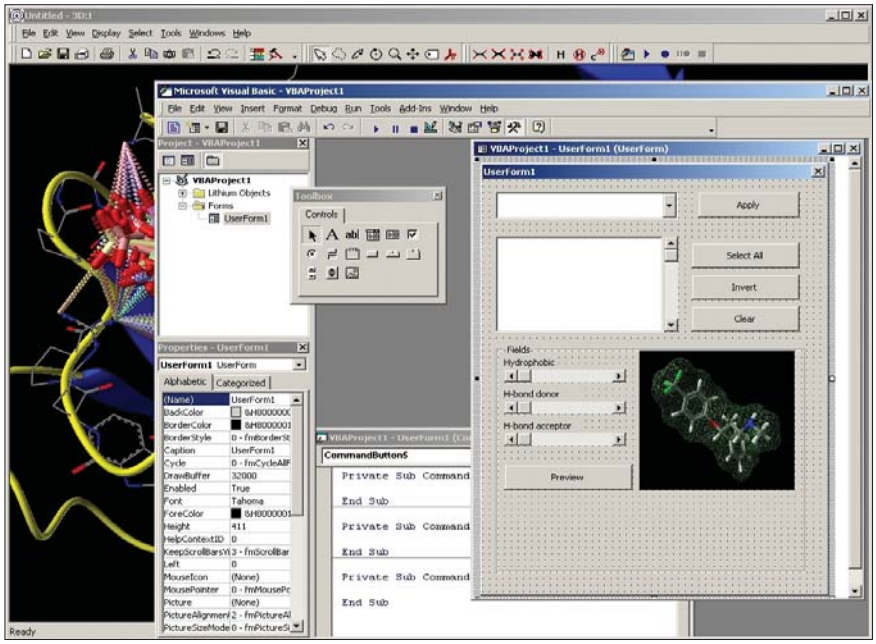
- Integration with Chemdraw sketcher for 2D molecular editing & sketching

Molecular Editing

- Live 3D views can be included within Powerpoint presentations for enhanced interactive communication
- 3D sketching for creation of new molecular structures
- Editing of existing molecular structures independently or in the context of proteins
- Full structure editing functions: atom/group addition, change atom/bond types, rotate bonds, invert chiral centers, auto minimization, measurement, extractions, etc.
- Intuitive interface — 3D editor is designed to be as similar as possible to sketchers commonly used by chemists (ChemDraw™, MDL® ISIS/Draw)

Communication

- Standard OLE copy and paste procedures with Windows-based productivity applications (Word, PowerPoint, Excel, Outlook, ChemDraw™, and MDL® ISIS/Draw)
- Sessions can be saved and emailed or otherwise distributed throughout an organization
- Reads and writes the same file formats as standard molecular modeling packages
- Publication quality rendering and printing; Direct saving of arbitrary size/resolution images in standard image formats
- Ability to save and add captions to viewpoints on molecular data
- Captioning with internal/external hyper-linkable text for Benchware 3D Explorer session and individual viewpoints with full text format control
- 3D annotation capability with full text format control
- Drag and drop capability for hypertext links (URLs) to Benchware 3D Explorer readable files



Using the Integrated Development Environment (IDE) for VBA, developers can rapidly create custom scripts, interfaces, and applications to address the specific needs of life sciences researchers. Custom-developed, task-based interfaces can shorten end user learning curves and leverage proprietary knowledge for strategic research advantage.

Development and Delivery

- All Benchware 3D Explorer functionality is accessible from VBA (279 classes, 2,645 methods and properties, 26 events)
- Well designed and comprehensive object model allowing fine control of the application from VBA scripts
- Spreadsheet, graphing, and web browser components accessible from VBA
- Macro recording and replay capabilities
- Chemical structure files and other data such as surfaces, fields, or VBA scripts can be loaded from remote machines using ftp or http protocols
- Benchware 3D Explorer COM components can be accessed from external programming languages such as Visual Basic, C++, C#, Python, or any other COM-enabled language
- VBA Integrated Development Environment (IDE) for rapid VBA code production

Hardware and Software Requirements

- Benchware 3D Explorer will run on PC hardware running Windows 2000 or XP (32 bit versions only). Minimum system configuration:
- Pentium III or Athlon 1.0 GHz processor or faster (1.5 GHz recommended)
- 128 MB of memory (256 MB recommended)
- 50 MB of free disk space
- Windows-compatible graphics card

Additional memory and processor speed will provide improved performance.

Hardware-accelerated OpenGL graphics hardware is required for optimal Benchware 3D Explorer performance.

Stereo-in-a-window viewing requires the use of specialized stereo glasses, an emitter, a stereo-capable graphics card, and a high refresh rate monitor (118Hz or better

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Benchware HTS DataMiner

Support for HTS Data Analysis

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Benchware® HTS DataMiner provides researchers with a high-capacity chemical spreadsheet environment and specialized modules to address specific research requirements. Chemical structures and chemical/biological data can be imported, joined from multiple sources, manipulated, and analyzed in an intuitive spreadsheet environment.

The base functionality of Benchware HTS DataMiner can be extended through two additional modules:

HTS Module - complete tools for the analysis of HTS and vHTS data through data mining algorithms (SAR Rules), and visualization and exploration of entire SAR landscapes (SAR Maps) including definition, management, and prioritization of chemical series for further research

HQSAR Module - rapid, automated QSAR technique for creation of predictive models and prioritization of chemical series from HTS data analysis

Base Functionality

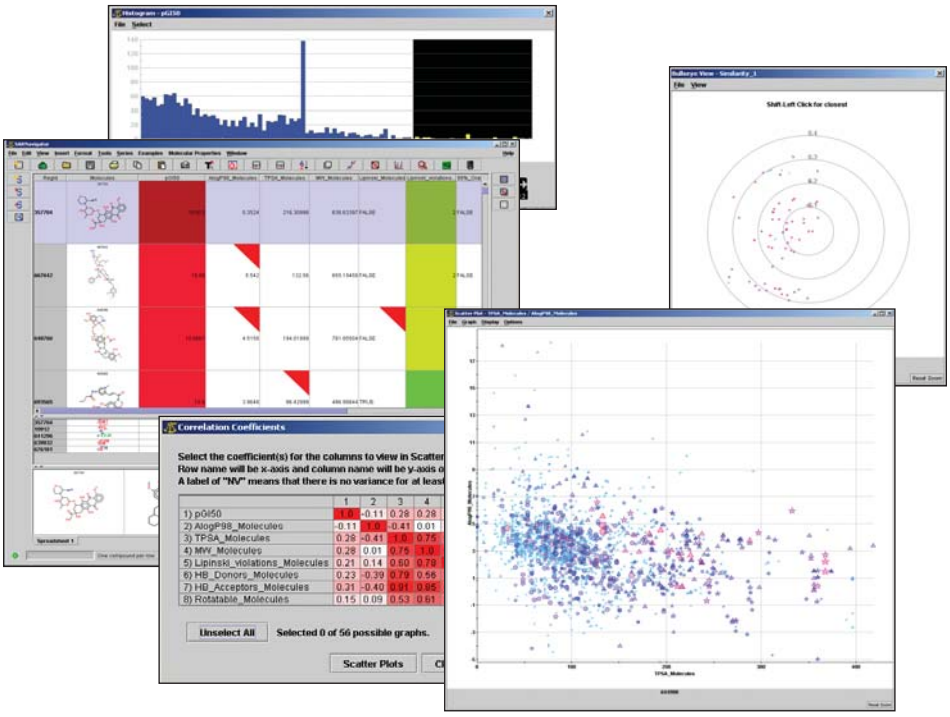
The base functionality of Benchware HTS DataMiner provides the chemical spreadsheet foundation for further modules of the Benchware HTS DataMiner system. The high-capacity, chemically aware spreadsheet processes molecular structures, enabling scientists to work interactively with large datasets such as those derived from High-Throughput Screening (HTS) and virtual High-Throughput Screening (vHTS) experiments. Chemical series creation, manipulation, and analysis tools allow users to deal simply with subsets of molecules within a broader chemical and biological context.

A wide variety of molecular descriptors can be computed and relationships within chemical-biological datasets investigated. Substructure search capabilities combined with maximal common substructure determination allow users to locate compounds containing a particular scaffold or undesirable molecular fragments. Researchers can view, compute properties, and analyze datasets of molecules as either whole molecules or as scaffolds and R-groups in an easily generated SAR table.

Base functionality can be utilized for decision support in medicinal chemistry, enabling researchers to understand relationships between biological activity and chemical structures. The base functionality of Benchware HTS DataMiner can be extended through the addition of other modules or through customization.

HTS Module

The HTS module of Benchware HTS DataMiner provides the functionality and workflow required to analyze the large results datasets produced from HTS and vHTS experiments. The HTS functionality has been designed and developed in conjunction with HTS data analysis groups at major pharmaceutical companies to address bottlenecks and challenges in HTS analysis procedures.



Data Exploration Capabilities
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 sceening data analysis.

Benefits

- Rapid identification of structurally similar, biologically active molecules from HTS data
- Comprehensive set of tools for the management, manipulation, and prioritization of chemical series for further research
- Prioritization of chemical series and prediction of biological activities based on statistically robust, rapidly calculable QSAR models

HQSAR Module

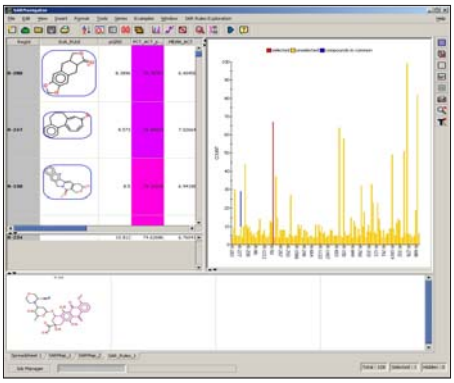
The HQSAR module of Benchware HTS DataMiner adds the ability to generate quantitative structure-activity relationship models to Benchware HTS DataMiner. Users can predict molecular properties or biological activity and highlight the molecular fragments important for that activity. Users can create and use their own QSAR models or share models with other Benchware HTS DataMiner users. The ability to create an explanatory HQSAR model on series of compounds derived from HTS screening results can be helpful in the prioritization of those series.

SAR Maps

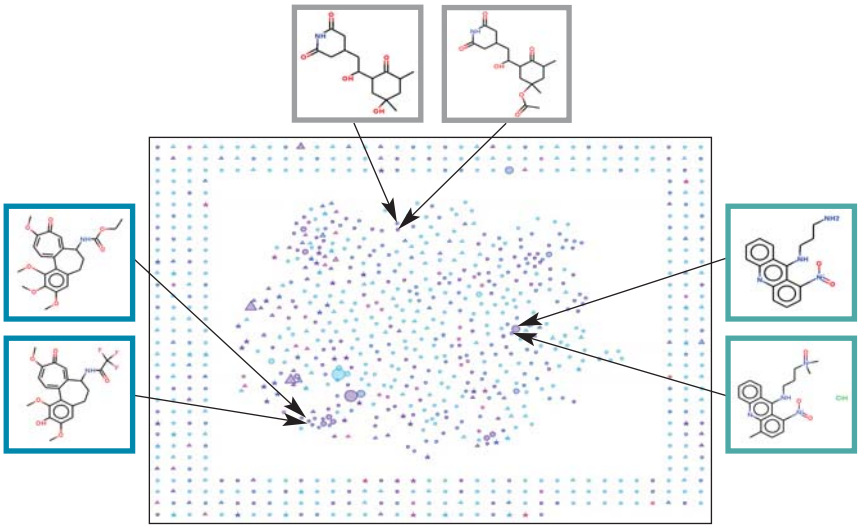
SAR Maps allow researchers to view and explore entire SAR landscapes from large-scale HTS, uHTS, and vHTS experiments incorporating both hit and similar non-hit compounds. SAR landscapes are viewed as 2D plots where compounds or clusters of compounds are plotted such that similar structures are in close proximity. Clustering, drill-down, and reprojection tools allow researchers to explore all areas of chemical information within a screening deck where a biological signal has been detected. Visualization of screening data through SAR Maps enables researchers to see the interrelationships of different chemical classes and allows simple, interactive identification and definition of chemical series for further research.

SAR Rules

SAR Rules technology allows researchers to rapidly mine HTS and vHTS data for groups of structurally related compounds that are highly enriched in hits. SAR Rules depict groups of connected molecular fragments that are found prevalently in screening hits and the compounds that contained those structural signatures. SAR Rules are generated through the Structural Units Analysis (SUA) algorithm and provide an automated method to determine groups of compounds that are the basis for chemical series. Users can control the number of compounds that a rule must contain as well as the nature and number of structural units that are examined. SAR Rules can be employed alone to determine chemical series or as a navigational aid to SAR Map data projections. Use of SAR Rules can also be used to analyze smaller groups of compounds such as project data to determine structural factors that lead to improved chemical and biological properties.



SAR Rules
SAR Rules data mining application within SARNavigator automatically determines scaffolds and substructures that elicit high biological activity. The sets of compounds found by SAR Rules provide an excellent starting point for the definition of chemical series for further research. SAR Rules take into account both active and inactive compounds and can be used as a navigational aid with SAR Maps.



SAR Landscape View
The HTS module employs SAR landscape views to allow users to visualize the entire biological signal found in the high-throughput screening deck. SAR landscape views are similarity plots where structurally similar compounds or clusters are plotted close in space. Biological activity, ADME, toxicology, selectivity, and other available data can be mapped onto plotted points guiding users to groups of chemical structures which possess the properties required to warrant further investigation. The ability to generate property statistics for clusters for landscape views, which include both hit and non-hit compounds, allows users to readily locate likely false negatives, false positives, and chemical series with highly sensitive SAR.

Series management tools in Benchware HTS DataMiner allow interesting chemical series to be captured, manipulated, and expanded once discovered. Defined chemical series can be prioritized for further research using molecular property profiles, SAR, or QSAR information. The combination of SAR Maps and SAR Rules provides Benchware HTS DataMiner with the most complete set of HTS analysis functions available in the industry. Using Benchware HTS DataMiner for HTS data analysis ensures the best possible decision about which compounds tested in HTS are worthy of secondary screening and further chemical exploration.

The results of HTS data analysis can be shared with other Benchware HTS DataMiner users allowing collaborative

Advantages

- Chemically aware spreadsheet environment with modular access to advanced tools ensures a consistent software research environment through HTS data analysis and beyond.
- Straightforward access to SAR views of data and a rapid QSAR technique ensure that datasets can be interactively examined for determinants of biological activity.

analysis. Chemical series defined in this way become initial SAR datasets to guide chemical synthesis decisions after secondary screening has confirmed biological activity.

Base Module Features

- High-capacity chemical spreadsheet
- Structure property calculation
- Chemical series management tools
- Substructure searching
- Creation of SAR tables through deconvolution of molecular structure into scaffold and R-groups
- Graphing with property mapping and data analysis tools

HTS Module Features

- SAR Maps - entire SAR landscape view of screening data through novel PCA/NLM procedure; macro recording and replay capabilities
- SAR Rules - rapid, flexible, automated identification of structurally related chemical series
- Interactive exploration tools for the analysis of large HTS datasets for use with both SAR Maps and SAR Rules
- Clustering, cluster analysis, and drill-down capabilities

Chemical series expansion capabilities to locate unscreened compounds suitable for inclusion in chemical series

HQSAR Module Features

- Rapid determination of predictive QSAR models
- Minimal requirement for user input
- Color coding of molecular structures to highlight important fragments

Validation

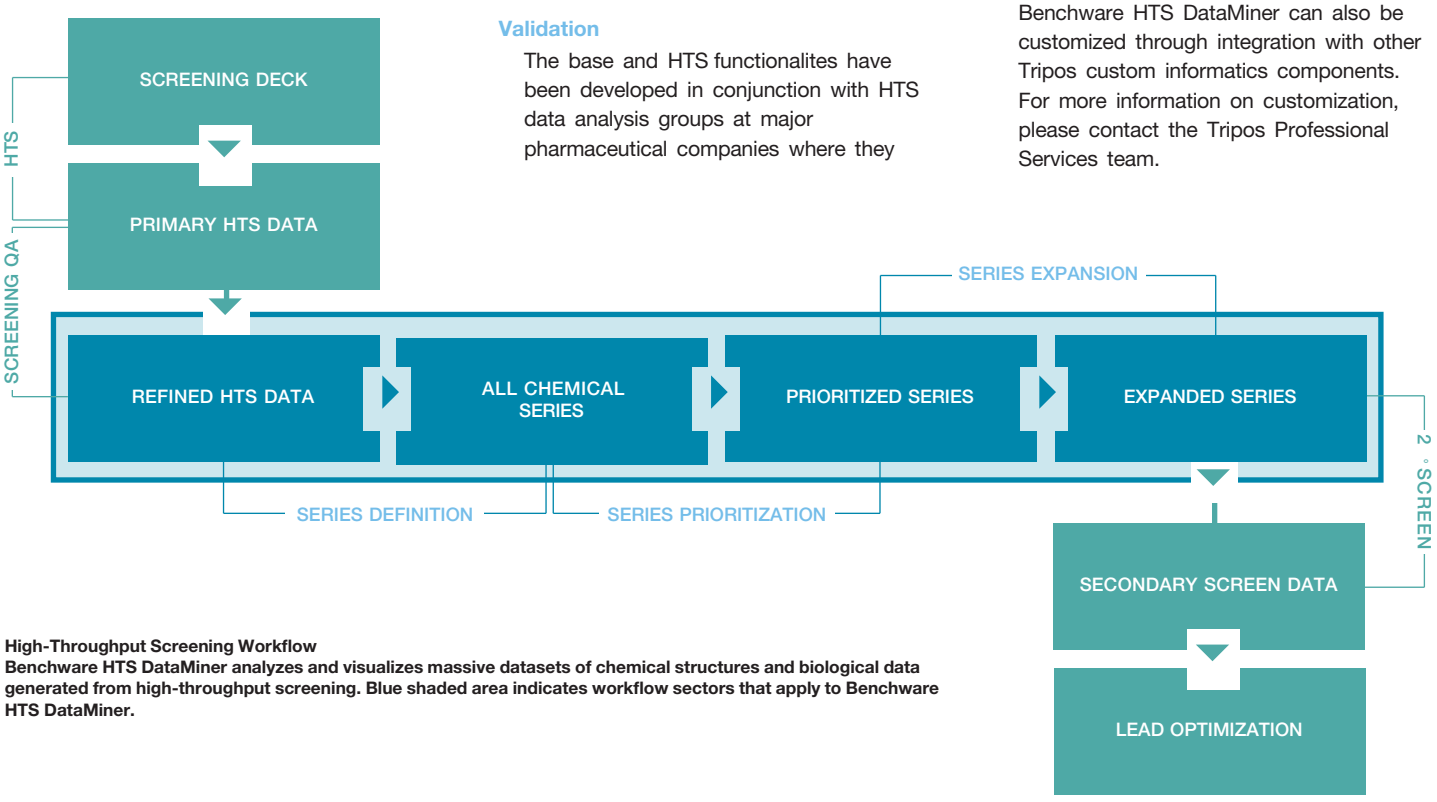
The base and HTS functionalites have been developed in conjunction with HTS data analysis groups at major pharmaceutical companies where they have been successfully employed to identify high-quality chemical series from HTS experiments for secondary screening and further chemical exploration. The HQSAR module utilizes the same underlying base code as the HQSAR module in the SYBYL® environment which has been extensively tested, validated, used, and published.

Customization

Benchware HTS DataMiner can be customized by Tripos or the user to address specific research goals and requirements. Two forms of customization are available:

- Jython scripting - for minor modifications, such as the computation of a new molecular property or column type, or implementation of new functionality
- Java services - for major customization, such as introduction of new data analysis modules

Benchware HTS DataMiner can also be customized through integration with other Tripos custom informatics components. For more information on customization, please contact the Tripos Professional Services team.



High-Throughput Screening Workflow
Benchware HTS DataMiner analyzes and visualizes massive datasets of chemical structures and biological data generated from high-throughput screening. Blue shaded area indicates workflow sectors that apply to Benchware HTS DataMiner.

Advantages *(continued)*

- HTS data analysis tools and processes allow the definition and prioritization of chemical series from views of the entire SAR landscape of an HTS screen including information from both hit and non-hit compounds.
- Customization capabilities allow ready incorporation of new science and workflow enhancements.

Hardware Requirements

Minimum system requirements are designed to allow complete functionality on collections of tens of thousands of compounds, and most functionality on collections of hundreds of thousands of compounds. Additional memory and disk space will provide maximum performance and the ability to process larger compound collections.*

Operating System

- Recommended: Windows® 2000 Service Pack 3 or Windows® XP
- Minimum: Windows® 2000 Service Pack 3 or Windows® XP

RAM

- Recommended: 512 MB
- Minimum: 384 MB

CPU Speed

- Recommended: 2.0 GHz
- Minimum: 1.0 GHz

Free Disk Space

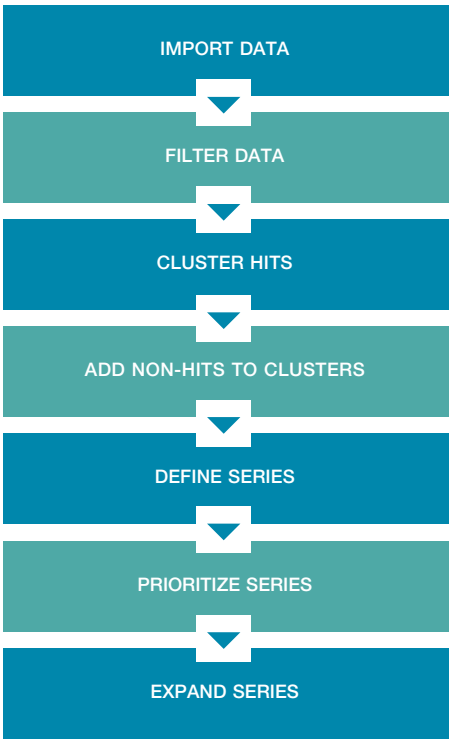
- Recommended: 2 GB
- Minimum: 500 MB

*Using Benchware HTS DataMiner with less than minimum system configuration will result in degraded software speed and performance.

Maximum Number of Compounds

- Recommended: Allows the use of all features on up to 15,000 compounds and Base module functionality on 200,000 - 300,000 compounds
- Minimum: Allows the use of all features on up to 2,000 compounds and the use of Base module features on up to 10,000 compounds

Benchware HTS DataMiner Analysis Process: Datasets can be analyzed in a variety of ways using Benchware HTS DataMiner. For high-throughput screening data analysis a process has been developed which allows researchers to explore the entire chemical information content of a screening deck where a biological signal has been found. By examining all compounds found to hit in a particular screen as well as similar compounds which were not hits, researchers can see all pertinent screening information with the minimum of computational overhead.



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Benchware Notebook

Scientific Planning, Documentation and Collaboration

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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 managment 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:

- Factiliates 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

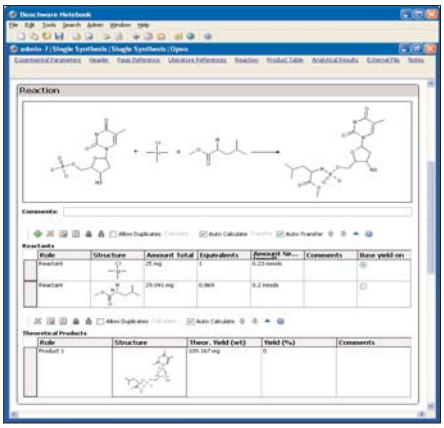
Benchware Notebook's fast search system allows arbitrarily complex queries to be quickly built and executed by end users. With all entered data stored in an underlying Oracle® database, Benchware Notebook users are able to dynamically search within their own notebook pages and pages of others across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