

Benchware

# 3D Explorer

## 3D Chemical Visualization and Decision Support



*Benchware® 3D Explorer empowers laboratory scientists to make more effective research decisions by allowing them to visualize, annotate, share and experiment with 3D chemical structures. Highest quality molecular graphics, user-friendly scientific tools, and integrated communication capabilities allow researchers to view, understand, and share complex molecular data such as protein-ligand crystal structures, docking results, molecular alignments, pharmacophores or other 3D chemical information. 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.
- Protein and ligand alignment capabilities allow rapid comparison of 3 dimensional properties.
- 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 hyper-linkable 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 inter-atomic bumps can also be visualized by strength, as well as prospective hydrogen bonding regions. 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 stereo.

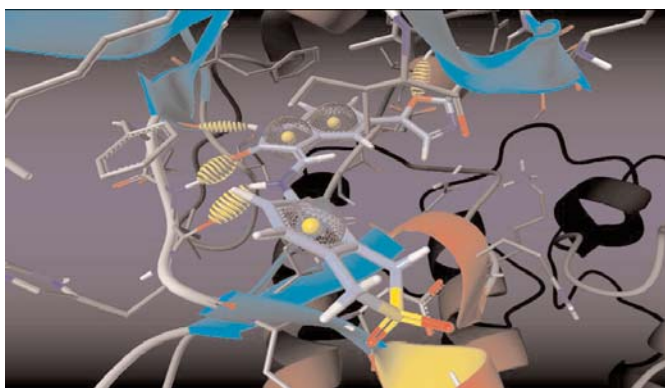
### Science Tools

Minimisation of molecular structures either alone or complexed with proteins is highly straightforward in Benchware 3D Explorer. Alignment of protein structures with their associated ligands allows comparison of

ligand interactions and understanding of selectivity. Automated rigid alignment of ligands puts new structural ideas immediately in the right molecular context and flexible alignment of ligands allows the understanding of structural similarity in 3D space. Molecular property calculations help determine the overall quality of new molecular ideas.

### 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 with on-the-fly calculated Lipinski properties.



PDB structure 1KE7 displayed in Benchware 3D Explorer depicts a potent, Oxindole-based CDK2 inhibitor. Hydrogen bonding interactions between the ligand and 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 by meshed spheres.

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## 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 (Symyx® Draw, ISIS®/Draw and ChemDraw™) 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.

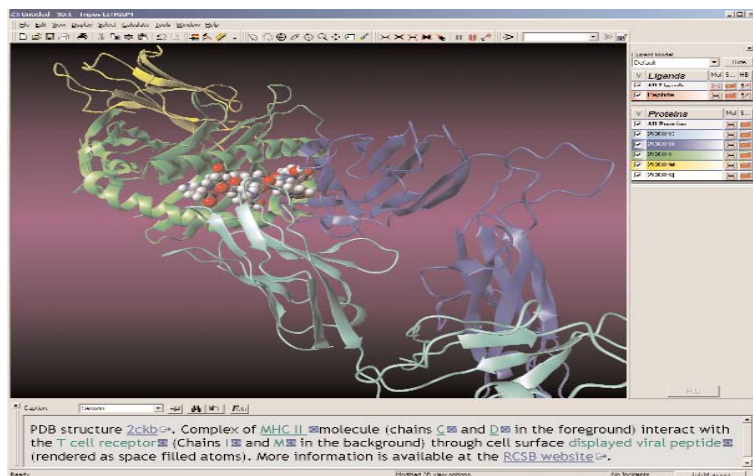
## Development and Delivery with Benchware 3D Explorer

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.

## Visualization

- Import and export a wide variety of chemical structure and related file formats (mol2, sdf, MDL mol, SMILES, PDB, etc.)
- Direct import from the RCSB crystal structure repository
- Visualize pharmacophores and 3D molecular queries
- Atom typing and configurable ligand extraction upon reading PDB files
- Cut & Paste structures from standard chemistry sketching packages (Symyx Draw, MDL ISIS/Draw, ChemDraw)
- State-of-the-art OpenGL graphics
- Standard molecular rendering styles (lines, capped sticks, ball & stick, space fill, tapered sticks)
- 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) with strength indication
- Comprehensive atom selection tools
- Hardware and side-by-side stereo-in-a-window 3D viewing capability (including support for Zalman LCD stereo monitors)
- Advanced display manager with ability to select structures, generate sub-groups, and create models



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.

## Communication and Integration

- Live 3D views can be included within PowerPoint presentations for enhanced interactive communication
- Standard OLE copy & paste procedure 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
- Cut & Paste structures from standard chemistry sketching packages (Symyx Draw, MDL ISIS/Draw, ChemDraw)
- Drag and drop capability for hypertext links (URLs) to Benchware 3D Explorer readable files

## 3D Explorer

## Science Tools

- Structure minimization of individual structures, complexes and ligands in the context of their host protein (Tripos or MMFF94s force fields)
- Protein structure alignment and molecular grouping
- Rigid-rigid alignment of small molecule structures with automated alignment on import
- Flexible alignment of small molecules to a template structure
- Tight integration with Symyx Draw and Chemdraw for 2D molecular editing & sketching
- Molecular property calculations

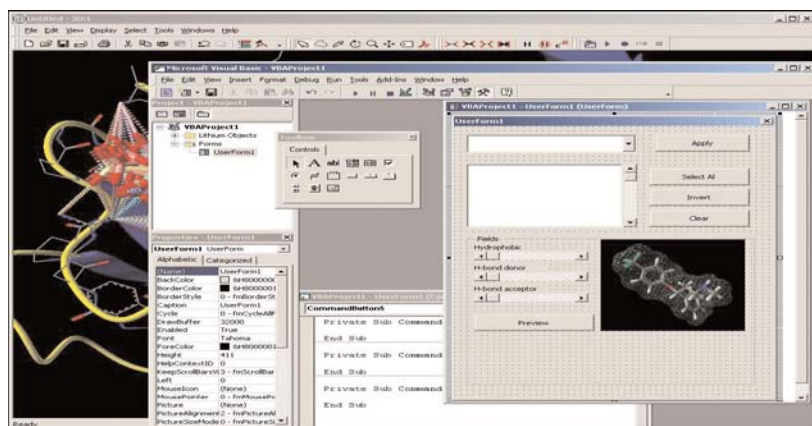
## Molecular Editing

- 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)
- On the fly calculation of Lipinski properties during 3D editing

## 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
- Included ActiveX control for integration into other applications
- VBA Integrated Development Environment (IDE) for rapid VBA code production



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.

## Custom Applications:

Many Benchware 3D Explorer users have built systems to allow researchers access to sources of 3D chemical information and published computational models. Such systems include:

- Access to in-house and public crystal structure database for chemical biologists
- Access to docking calculations for medicinal chemists
- Access to advanced alignment and pharmacophore tools
- Access to CADD produced computational models (UNITY, Docking, Metasite...)

## 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.

## Benchware® DataMiner

Benchware DataMiner is ideal for analysis of large and small biochemical datasets. DataMiner provides an unparalleled set of SAR analysis capabilities including novel SAR Map and SAR Rules capabilities for rapid (v)HTS data analysis.

## System Requirements

Benchware 3D Explorer will run on PC hardware running Windows XP or VISTA (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 recommended) or use of the Zalman stereo LCD.

Download a free 30-day evaluation:

[www.tripos.com/download](http://www.tripos.com/download)

Registration required