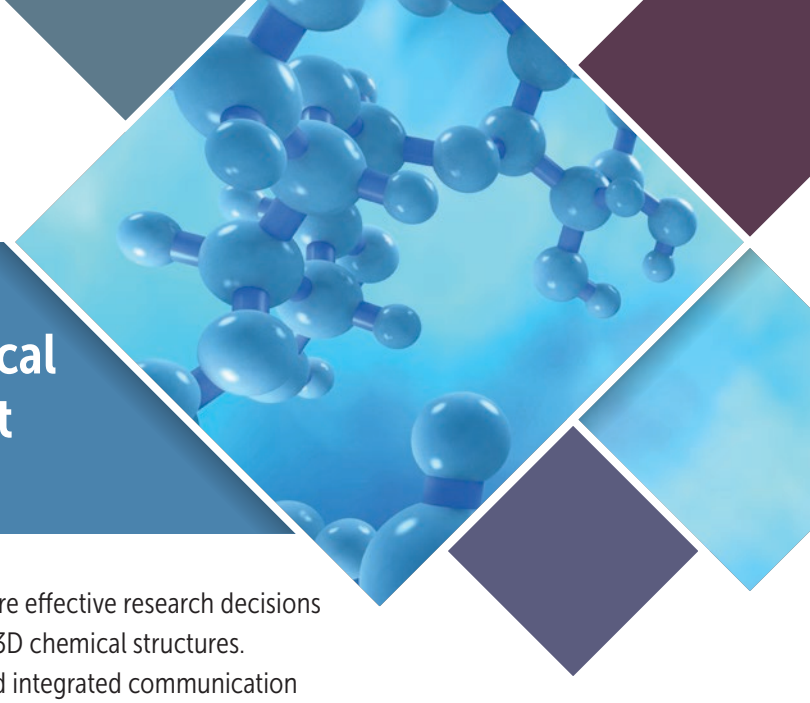
CERTARA



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.

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

Minimization 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 Benchware Key Benefits 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.

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

(continued)

Key Benefits

- 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 return on investment 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

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.

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 and 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 and stick, space fill, and 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 subgroups, and create models

Communication and integration

- Live 3D views can be included within PowerPoint presentations for enhanced interactive communication
- Standard OLE copy and 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 hyperlinkable text for Benchware
- 3D Explorer session and individual viewpoints with full text format control
- Cut and 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

Science tools

- Structure minimization of individual structures, complexes and ligands in the context of their host protein (Certara 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 and 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

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 and Metasite)

Complementary offerings

SYBYL-X

SYBYL-X'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.

D360 for discovery

The D360 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.

System requirements

Benchware 3D Explorer will run on PC hardware running any of the following operating systems:

- Windows 7 (32 or 64 bit)
- Windows Vista (32 bit versions only)
- Windows XP

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.

About Certara

Certara is a leading provider of decision support technology and consulting services for optimizing drug development and improving health outcomes. Certara's solutions, which span the drug development and patient care lifecycle, help increase the probability of regulatory and commercial success by using the most scientifically advanced modeling and simulation technologies and regulatory strategies. Its clients include hundreds of global biopharmaceutical companies, leading academic institutions and key regulatory agencies.

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