

# DISCOVERY STUDIO<sup>®</sup> VISUALIZER 3.1



If you need access to commercial-grade 3D molecular visualization tools for viewing, sharing and analyzing protein and small molecule data, then Discovery Studio Visualizer (DS Visualizer) offers an extensive set of free functionality

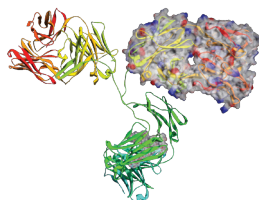
DS Visualizer is a free, feature-rich molecular modeling environment, for both small molecule and macromolecule applications. Built from, and fully compatible with the latest release of our enterprise-ready expert modeling product, Discovery Studio 3.1, experts and colleagues can seamlessly and efficiently exchange results, without loss of either time or scientific information

## DISCOVERY STUDIO VISUALIZER

With Discovery Studio Visualizer (DS Visualizer), the following features are available without a license:

### • Visualization:

- Advanced molecular visualizations
- Publication quality graphics
- Hardware acceleration and stereo support<sup>†</sup>



### • Macromolecule design:

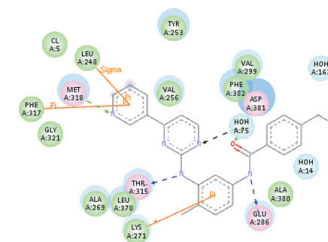
- View and edit multi-domain protein sequences (e.g., Antibodies)
- Predict Secondary structures
- Superimpose and edit protein structures

### • Ligand-based design:

- Sketching and fragment building tools
- Manual pharmacophore generation
- Flexibly overlay ligands

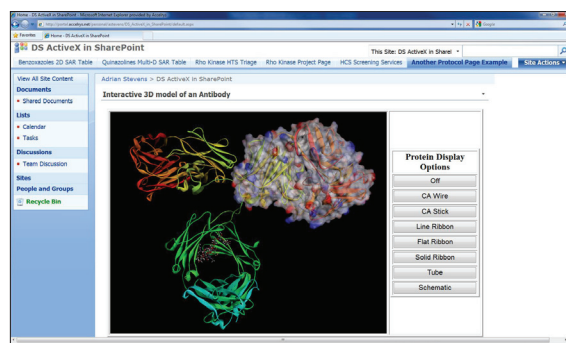
### • Structure-based design:

- Define, display and edit ligand binding sites
- Create 2D ligand-receptor interaction diagrams
- Monitor key H-bonds, Pi-Pi, Cation-Pi, and Sigma-Pi interactions



### • Share and Collaborate:

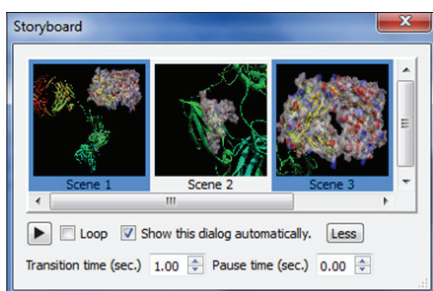
- Visualize 3D molecules in Microsoft Office<sup>®</sup> and web pages (ActiveX Control)
- Capture and share scenes with 'Storyboard'
- Access 2D and 3D charts, heat maps and more



## NEW IN DS VISUALIZER 3.1

The latest release of Discovery Studio Visualizer includes a number of new enhancements:

- **Storyboard playback and Timings:** Storyboards can now be played as a movie, with options for setting transition and pause times. You can also set the dialog to open automatically whenever a .DSV file containing a storyboard is opened.



- **Export as movie:** Storyboards can now be exported as .webM movies.
- **Save As html:** Save 3D molecules directly into a single html file. Easily share or upload to websites and Microsoft™ SharePoint™.
- **Save As PPT slide:** Simplify the process of creating presentations containing your 3D molecules by directly creating a Microsoft PowerPoint™ slide.

## UPDATED! DS3.1 ACTIVEX CONTROL

DS ActiveX Control is a free plug-in\* that provides interactive 3D visualization of small molecules, proteins, nucleic acids, crystal structures and pharmacophore models. Our latest release of the web tool has been completely revised and updated. New features include:

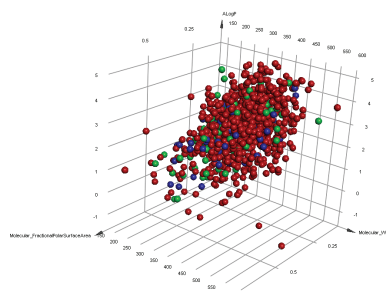
- **Storyboard support:** Incorporates all of the scene transition, timing and auto-play features.
- **DSV file support:** Now fully supports the latest release of the Accelrys DSV file format.
- **Graphics support:** Supports the latest enhancements to depth blur, and also direct and ambient shading.

\* DS ActiveX Control is an independent product and is available as a separate free download with DS Visualizer. It does not require the installation of DS Visualizer.

## MOLECULAR VISUALIZATION

DS Visualizer provides functionality for visualizing, analyzing, and sharing biological and chemical data. It allows you to view molecular data from multiple perspectives by providing the options to view data through 3D structures, sequences, and data tables.

- **Interact** with and rapidly analyze your data using the Molecule Window, which supports visualization, data table and hierarchy views of the data.
- **View** and manipulate publication quality 3D molecular structures ranging from atomic-level to large macromolecular complexes.
- **Generate** a variety of charts such as 3D point plots, heat maps and Ramachandran plots to analyze your data.



- **Scroll** through sets of molecules with the help of navigation keys, easily managing complex libraries.
- **Manage** large data sets with ease using the integrated browser in the Molecule window. Visualize structures in different colors by property of interest.
- **Study** multiple chain proteins and nucleic acids using the sequence window. View sequences and alignments for sequence to structure comparisons, sequence annotations and sequence family analysis.



## Supported Operating Systems†

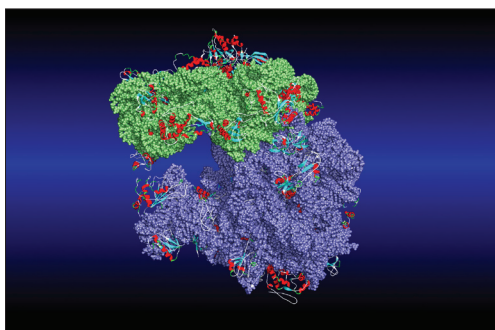
Windows and Linux compatible:

- **Windows:** XP, Vista (32bit), Windows 7 (64 bit)
- **Linux:** Red Hat 4 (32/64 bit), Red Hat 5 (64 bit) and SUSE 10, 11 (64 bit)

## DISPLAY AND GRAPHICAL OUTPUT

The DS Visualizer outputs high quality graphics ready to be used for slideshows, posters, or any other presentation format.

- **Graphics Performance:** The Visualizer makes use of advanced hardware acceleration to improve handling of very large macromolecule systems.
- **Shading and Depth Blur:** Generate ambient and direct shadows, depth blur, atom contouring and custom backgrounds.
- Control lighting, depth cueing and graphics quality to enhance visualization.
- Augment 3D structure appearance with multisided surfaces and isosurfaces and apply material appearances (e.g., metallic or plastic) to create graphics that are polished, professional and ready for presentation.
- Export jpg, .jpeg, .bmp and .png files.
- Save high quality 3D graphics as POV-Ray files.



## Supported Graphics Cards†

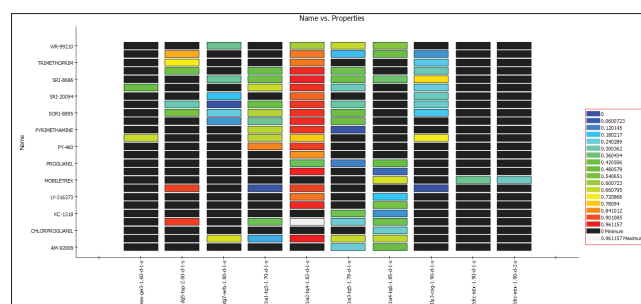
The following cards are supported with both DS3.1 and DS Visualizer 3.1:

- **ATI FireGL** V3600, V5600, V7600[St], V7700[St], V8600[St]
- **ATI FirePro** V3800, V5800, V8700[St]
- **NVidia Quadro** FX 570, 580, 1800, 3800[St], 4600[St], 4700[St], 4800[St], 5600[St], 5800[St]

## IMPORT, BUILD AND ANALYZE STRUCTURES

DS Visualizer can handle a range of data types, including 2D and 3D structures. You can even download structures and sequences directly from the PDB, or NCBI.

- Sketch, build and modify 3D structures using sketching and fragment building tools.
- Superimpose structures based on tethers, residues or sequence alignment
- Build pharmacophore models to visualize properties such as hydrophobicity, hydrogen bond donors and acceptors and aromatic rings.
- Manually derive pharmacophore models from small molecules or protein-ligand complexes.
- Visualize properties of large sets of molecules with a user-defined color scheme.
- View molecular data in multiple perspectives such as 3D structure, sequence, chart/graph and table.
- Alter geometric and chemical properties and monitor structural orientations and interactions
- Calculate solvent accessibility, RMSD and predict secondary structures within a single environment.



## CUSTOMIZATION

DS Visualizer can be customized to suit your workflow:

- Add toolbars, buttons and shortcut keys.
- Dock and undock tabbed windows from the main application.
- Drag and drop files from your desktop or file explorer.
- Use Perl scripting to automate common workflows.

† Further information is available at [accelrys.com/products/discovery-studio/requirements/technical-requirements-310.html](http://accelrys.com/products/discovery-studio/requirements/technical-requirements-310.html)

## DISCOVERY STUDIO 3.1 VISUALIZER: FREE VERSUS COMMERCIAL COMPARISON

- Free DS Visualizer: In 'Visualizer' mode, a limited set of functions from the licensed Discovery Studio client are available. For example, you can view and edit molecular structures, sequences and sequence alignments and even perform basic molecular overlays. You can also automate tasks using a subset of the DS Perl API.
- Full Discovery Studio: With the addition of a license, the Visualizer client runs in full mode.

- Connect to an existing Pipeline Pilot server
- Access Discovery Studio protocols available in Pipeline Pilot for protein design and analysis, structure-based design, pharmacophore modeling, ADMET predictions and simulations
- View and customize protocols, share them with colleagues, and run them from the Discovery Studio or Pipeline Pilot client

To learn more about Discovery Studio, go to:

[accelrys.com/discovery-studio](http://accelrys.com/discovery-studio)

Type	Feature	DS Visualizer	DS Client
Client	Supported on Windows 7, Vista, XP and Red Hat Linux 4.0, 5.0, and SUSE 10 <b>New!</b>	✓	✓
	Welcome Page with quick access to files and information	✓	✓
	Custom short-cut keys and toolbars	✓	✓
	Perl scripting	✓	✓
	Files explorer view	✓	✓
	Table browser for small molecule data sets	✓	✓
	Protocols, jobs, parameter help, and tools explorer views	✓	✓
General	Unified Molecule Window with 3D view and associated hierarchy and data table views	✓	✓
	Create multiple sided surfaces and isosurfaces for enhanced molecular visualization	✓	✓
	Access to charts, including 2D (line and point), 3D point plots, heat maps, histograms and more <b>New!</b>	✓	✓
	Force field typing for generation of parameter and topology files used in molecular simulations <b>New!</b>	✓	✓
	Constraints and restraints setup for molecular simulations <b>New!</b>	✓	✓
	Molecular Dynamics Simulations †	✓	✓
	Superimpose structures based on tethers, residues, sequence alignment <b>New!</b>	✓	✓
	Superimpose structures based on molecular overlay functionality	✓	✓
	RMS calculations	✓	✓
	Transformation matrix and center of geometry	✓	✓
	Calculate basic molecular properties <b>New!</b>	✓	✓
	Launch protocols from the toolbar †	✓	✓
	Protein	Molecular Builders for peptides and nucleic acids <b>New!</b>	✓
Access to Side-Chain Rotamer conformations and interaction analysis <b>New!</b>		✓	✓
Structure superimposition by alignment <b>New!</b>		✓	✓
Structure and Sequence alignment †		✓	✓
Support for a variety of sequence-structure formats		✓	✓
Sequence windows		✓	✓
Secondary structure prediction		✓	✓
Graphing functionality, including Ramachandran and contact plots <b>New!</b>		✓	✓
Contour and display X-ray electron density maps		✓	✓
3D pointer to navigate structures and place 3D labels <b>New!</b>		✓	✓
Basic tools to edit X-ray structures <b>New!</b>		✓	✓
Build and refine X-ray Structure		✓	✓
Place and refine X-ray Ligand Structure		✓	✓
Ligand Design	Dendrogram toolbar	✓	✓
	Access protocols to prepare, minimize and refine protein structures, generate protein reports and validate protein structures †	✓	✓
	View two-dimensional chemistry	✓	✓
	Sketch 3D molecules	✓	✓
	Modify or build custom 3D small molecules using a tool panel of pre-defined fragments <b>New!</b>	✓	✓
	Type atoms to prepare molecules prior to energy calculations <b>New!</b>	✓	✓
	Modify conformations using a tool panel to perform Dreiding minimization, coordinate kick, and torsion kick	✓	✓
	Analyze molecular dynamics trajectories based on RMSD, close contacts and hydrogen bonds	✓	✓
	Calculate molecular energy and perform energy minimization using CHARMM force field †	✓	✓
	Analyze complexes <b>New!</b>	✓	✓
	Monitor Pi-Pi, Cation-Pi, and Sigma-Pi interactions	✓	✓
	Generate 2D receptor-ligand interaction plots <b>New!</b>	✓	✓
	Define, display and edit ligand binding sites <b>New!</b>	✓	✓
Manually generate pharmacophore (Catalyst) queries	✓	✓	
Automatically generate and analyze pharmacophore models	✓	✓	

† Note: Running protocols does require additional product licensing from Accelrys.