Visualization in Discovery Studio

Molecular visualization is a key aspect of data analysis that can provide understanding about the implications of a molecule's structure on certain interactions and biochemical reactions, while often divulging mechanistic insight about a biochemical pathway or lead compound. Many sophisticated visualization tools are available in Discovery Studio® (DS), which is a Windows- and Linux-based research environment that delivers a comprehensive suite of modeling and simulation solutions for protein modeling, receptor-ligand interactions, simulations, pharmacophore modeling and computational chemistry.

Discovery Studio Visualizer Pro

DS Visualizer Pro provides functionality for visualizing, analyzing and sharing biological and chemical data. DS Visualizer Pro allows molecular data to be viewed from multiple perspectives by providing the options to view data through 3D structures, sequences, charts/graphics and data tables.

- All of the windows associated with molecular data, such as the 3D, sequence and chart windows, are interconnected to allow for interactive selection for rapid and simplified analysis of your data.

Structure Importing, Building and Analysis

Discovery Studio is a very flexible environment that allows data to be transferred and analyzed in multiple formats. Several file formats for 3D structures, SMILES, sequences and graphics are supported. Structures and sequences can be accessed and imported directly from the PDB or NCBI. DS Visualizer Pro includes many tools that allow you to edit your structure and perform calculations to help you gain further insight into its molecular properties.

- Your 3D structures can be easily sketched, built, and modified with sketching and fragment builder tools.
- The interactive environment allows you to alter geometric and chemical properties, as well as monitor structural orientations and interactions.
- Molecules can be typed with specific forcefields for analyzing molecular mechanics and viewing multiple conformations and minimized structures.
- DS Visualizer Pro includes tools for calculating solvent accessibility and RMSD, identifying binding sites, superimposing structures, and predicting secondary structures.

With these tools, acquiring, building and analyzing molecular structures is convenient, straightforward and well suited to meet your visualization and analysis needs.
Customization and Scripting

Discovery Studio helps streamline your workflow by letting you tailor the environment to fit your personal preference and needs. The interface can be customized by adding user-defined toolbars and buttons, tool panel layouts, shortcut keys, and modifying default parameter settings; your unique customized user interface will then persist for each session.

- You can simplify your workflow by dragging and dropping files from your desktop or file explorer window directly into DS Visualizer Pro.
- You can automate your molecular manipulation workflows through Perl scripting via either the command-line or DS Visualizer Pro client.

Display and Graphical Output

Once you are ready to present your results, DS Visualizer Pro will allow you to change the display style of molecular, sequence or graphical data and output high quality graphics that are ready for slideshows, posters, or anything else you need.

- You can control lighting, depth cueing, and graphics quality to enhance visualization.
- You have the ability to augment 3D structure appearances through multi-sided surfaces and isosurfaces, and apply material appearances (e.g. metallic or plastic surfaces) to help your graphics look polished, professional, and ready to be presented.

DS Visualizer Pro Enterprise

The DS Visualizer Pro Enterprise version provides all the same functionality as DS Visualizer Pro, and also serves as the single interface for easily accessing all the expert-level life science modeling and simulation software that is available in Discovery Studio, as well as shared custom protocols.

- Because Discovery Studio is built upon the SciTegic Enterprise Server platform, the DS Visualizer Pro Enterprise can accommodate the integration of scientific components developed by Accelrys, as well as components developed by other third-party software vendors or your own organization. Accelrys’ Client Services group can help you integrate all the tools you need in order to streamline your workflow and make your research processes more efficient.
- The underlying server platform also enables integration between Discovery Studio and SciTegic Pipeline Pilot, meaning you can quickly access protocols for ADMET, analysis, protein modeling, receptor-ligand interactions, pharmacophore modeling and simulation through either the Discovery Studio or Pipeline Pilot interface.
- With the DS Visualizer Pro Enterprise version you have access to protocols for preparing ligands and converting interactions to features.
- With the Pipeline Pilot professional client interface, you can view and customize protocols, share them with your colleagues, and run them in either the Discovery Studio or Pipeline Pilot interface.

Organizational Scheme

DS Visualizer Pro conveniently stores, searches and organizes your files, experiments, protocols, jobs, and tools in customizable and flexible ‘Explorer’ views.

- The Files Explorer allows you to quickly store, retrieve, and manage data, scripts and experiments saved in your file system or mounted drives. In addition, history and sample data can be quickly accessed.

- Pre-built scientific or custom protocols located in the Protocols Explorer* are organized by functionality into folders containing protocols for ADMET descriptors, protein modeling, simulations, analysis, receptor-ligand interactions, and pharmacophore modeling, as well as your personal user folder to store custom built or favorite protocols.

  *Protocols Explorer only available in DS Visualizer Pro Enterprise.

- The Tools Explorer allows for quick access to common actions for manipulating and analyzing your molecular data—such as editing and analyzing pharmacophores, applying constraints, building fragments, modifying conformations, analyzing trajectories, and performing forcefield typing and binding site analysis.

Required Software

DS Visualizer Pro Enterprise (or DS Visualizer Pro with Pipeline Pilot Server)

Loop refinement (protocol) and protein validation (Protein Health tool panel) was performed on a protein model generated from a sequence with unknown structure. The stick representation of the best loop is shown.