Enhanced communication, collaboration, and understanding across scientific disciplines

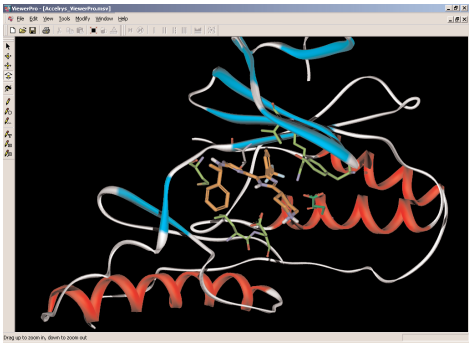
Fully Windows integrated, 3D molecular visualization and chemical communications software

Provides powerful insight into chemical functionality that is responsible for ligand-receptor binding affinity

Discovery Studio Datasheet

DS ViewerPro

Experimental chemists, computational specialists, and biological scientists alike can benefit from visualizing and sharing molecular information using Discovery Studio™ ViewerPro. Communication, collaboration, and understanding across scientific disciplines can be enhanced with the DS ViewerPro's consistent representation of molecular structures, whether they are small organic molecules, proteins, or crystalline structures. DS ViewerPro is part of Accelrys' Discovery Studio family of products that include a knowledge management system built on a common technology platform that offers easy interaction with varied corporate databases and simple transfer of information between modules, applications, users, and workgroups.



▲ *The DS Viewer's flexibility in creating visual rendering was used to highlight the active site in this protein-ligand complex.*

Visualization

The DS ViewerPro provides access to flexible visual rendering options. You can interactively rotate and scale molecules and apply a wide variety of display styles to highlight key structural features. The wide variety of visualization and rendering controls allow you to custom tailor the appearance of your model for maximum effectiveness.

Modules

The utility of DS ViewerPro is further increased with a number of add-on modules that extend its computational capability. DS ViewerPro add-on modules include a property calculator for calculating molecular properties, a conformer generator that suggests alternative conformations, and molecular overlay which provides techniques for molecular superimposition.

Communication

Effective transfer of knowledge between computational and desktop environments relies on consistent representation of data. The DS ViewerPro can read files from other modeling applications as well as public data sources like the Protein Data Bank. Once information is in the desktop environment, the DS ViewerPro can be used to integrate molecular models with other productivity applications.

You can use e-mail to send molecules from within the DS ViewerPro using the File/Send command. Use the Open Location command to load files from remote computers anywhere on your corporate intranet or the Internet.

Analysis

Analysis and measurement tools help you to evaluate geometry and understand chemistry. DS ViewerPro automatically calculates a handful of basic atomic and molecular properties for molecules sketched or read in. Measurement monitors can be created, all of which are completely dynamic. As your modeling environment changes, your monitors are automatically recalculated. Additional analysis features include tools for investigating potential hydrogen bonds or computing solvent-accessible surface area.

Accessing Data

In addition to the highly interactive 3D view, DS ViewerPro provides two other ways to 'see' and interact with your data.

Hierarchy Window

The Hierarchy Window shows object relationships

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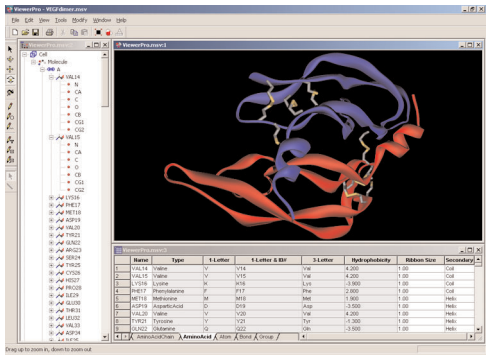
within your model by providing alternate ways to view your model. For example, you can view the atoms that make up individual amino acids, a polypeptide chain, or an entire protein.

Data Table

All of the properties within a molecular system can be accessed through the spreadsheet view called the Data Table Window. In this window, all properties for each type of molecular object are accessed via separate tabbed views. For example, all atoms and their properties are viewable within a separate tabbed view labeled 'Atoms.' Each row represents a unique object (molecule, atom, amino acid, etc.) with all of its properties organized into the appropriate columns.



Integration

OLE Embedding Molecule Objects

The DS ViewerPro products are capable of interacting with other Object Linking and Embedding (OLE) compliant software. This adds the ability to display, edit, or embed molecules within other programs such as word processing or presentation software. To embed a molecular object from the DS ViewerPro, simply use the Copy command from the Edit menu and paste into another application.

Web Browser Integration

The DS ViewerPro's integration capabilities have been extended to include html browser-based interaction. With the DS ViewerPro working as a helper application, structures can be accessed and manipulated from a web page. Images can also be created for delivering web-based content.

Discovery Studio: Integrated Platform for Drug Research

DS ViewerPro is a component of Discovery Studio, Accelrys' software architecture specially designed for the unique requirements of the pharmaceutical and biotechnology industries. This emerging suite of informatics, modeling, and simulation tools provide great science from easy-to-use desktop software that interacts with the databases throughout the corporate IT infrastructure. As a result, chemists and biologists realize better collaboration and R&D workflow because they can seamlessly transfer information between modules, applications, users, and workgroups.

Like DS ViewerPro, Discovery Studio desktop tools are built upon the popular, well-established Windows® operating system, making it easier for scientists who are new or occasional users of computational tools to learn and use them to their potential. Being Windows-based also facilitates the quick transfer of analysis results to desktop productivity tools for further study or for communicating findings with colleagues.

Through its integrated project knowledge management system (DS ProjectKM), Discovery Studio provides the navigation and searching tools through which scientists gain quick access to data stored in Oracle® relational databases. R&D productivity improves as a result of easier collaboration and sharing of information between the various groups involved in the drug discovery process.

Discovery Studio's computational and data management tools will aid every aspect of drug development. Its modular plug-and-play architecture will make for fast incorporation of new Accelrys' applications as they are delivered into the Discovery Studio environment. In addition, third-party and in-house tools can be integrated into its flexible framework to achieve a tailored enterprise system.

System Requirements

DS ViewerPro runs on Windows® 98, NT, and 2000 PCs.

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