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# **Introduction to Biovia Discovery Studio**



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# Introduction

- **Discovery Studio** is a suite of software for simulating small molecule and macromolecule systems. It is developed and distributed by Dassault Systemes BIOVIA (formerly Accelrys).
- It is a comprehensive software suite for analyzing and modeling molecular structures, sequences, and other data of relevance to life science researchers.
- The product includes functionality for viewing and editing data along with tools for performing basic data analysis.
- The Discovery Studio Visualizer is a free viewer that can be used to open data generated by other software in the Discovery Studio product line. It is designed to offer an interactive environment for viewing and editing molecular structures, sequences, X-ray reflection data, scripts, and other data.



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- It also provides a rich set of viewers for displaying plots and other graphical representations of data. The application runs on Windows and Linux and is a fully integrated desktop environment that provides access to standard operating system features such as the file system, clipboard, and printing services.

## Scope

Discovery Studio provides software applications covering the following areas:

- **Simulations**

- Including Molecular Mechanics, Molecular Dynamics, Quantum Mechanics
- For molecular mechanics based simulations: Include implicit and explicit-based solvent models and membrane models



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- Also includes the ability to perform hybrid QM/MM calculations
- **Ligand Design**
  - Including tools for enumerating molecular libraries and library optimization
- **Pharmacophore modeling**
  - Including creation, validation and virtual screening
- **Structure-based Design**
  - Including tools for fragment-based placement and refinement, receptor-ligand docking and pose refinement, de novo design
- **Macromolecule design and validation**



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- **Macromolecule engineering**
  - Specialist tools for protein-protein docking
  - Specialist tools for Antibody design and optimization
  - Specialist tools for membrane-bound proteins, including GPCRs
- **QSAR**
  - Covering methods such as multiple linear regression, partial least squares, recursive partitioning, Genetic Function approximation and 3D field-based QSAR
- **ADME**
- **Predictive toxicity**



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➤ This application starts by clicking on the icon on the Desktop.

Discovery Studio Visualizer

File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help

Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools

Search product features

Tools x DS Welcome x

BIOVIA | Discovery Studio 2017R2

What's new

Actions

My Recent Actions

- ▶ Open URL...
- ▶ Open...

My Recent Tool Panels

As you access different tools, the most recently used tool panels will be listed here.

Data

My Recent Files

- ▶ 3rze receptor.dsv
- ▶ 3rze.pdb
- ▶ Famotidine 1.dsv
- ▶ 6icg ALXR.dsv
- ▶ Aspirin.dsv
- ▶ 6icg.pdb
- ▶ 5u09 Cannabinoid.dsv
- ▶ 5u09.pdb
- ▶ 5xr8.pdb
- ▶ Paracetamol.dsv
- ▶ 4orrH2 receptor.dsv
- ▶ 4orr.pdb
- ▶ Famotidine.dsv
- ▶ 3bbb.pdb
- ▶ 5tgz Cannabinoid.dsv

Upgrade

▶ Upgrade now

Want more Discovery Studio? Unleash the power of the complete Discovery Studio with the BIOVIA Foundation:

- Homology Modeling
- Model Antibodies
- Create Pharmacophores
- Search and Build Databases
- Docking
- Fragment Based Design
- Scoring and Analysis
- Dynamics
- Electrostatics
- QM-MM
- ADMET
- Conformations
- Library Analysis and Design
- QSAR/SAR
- And more!

Enable Additional Features

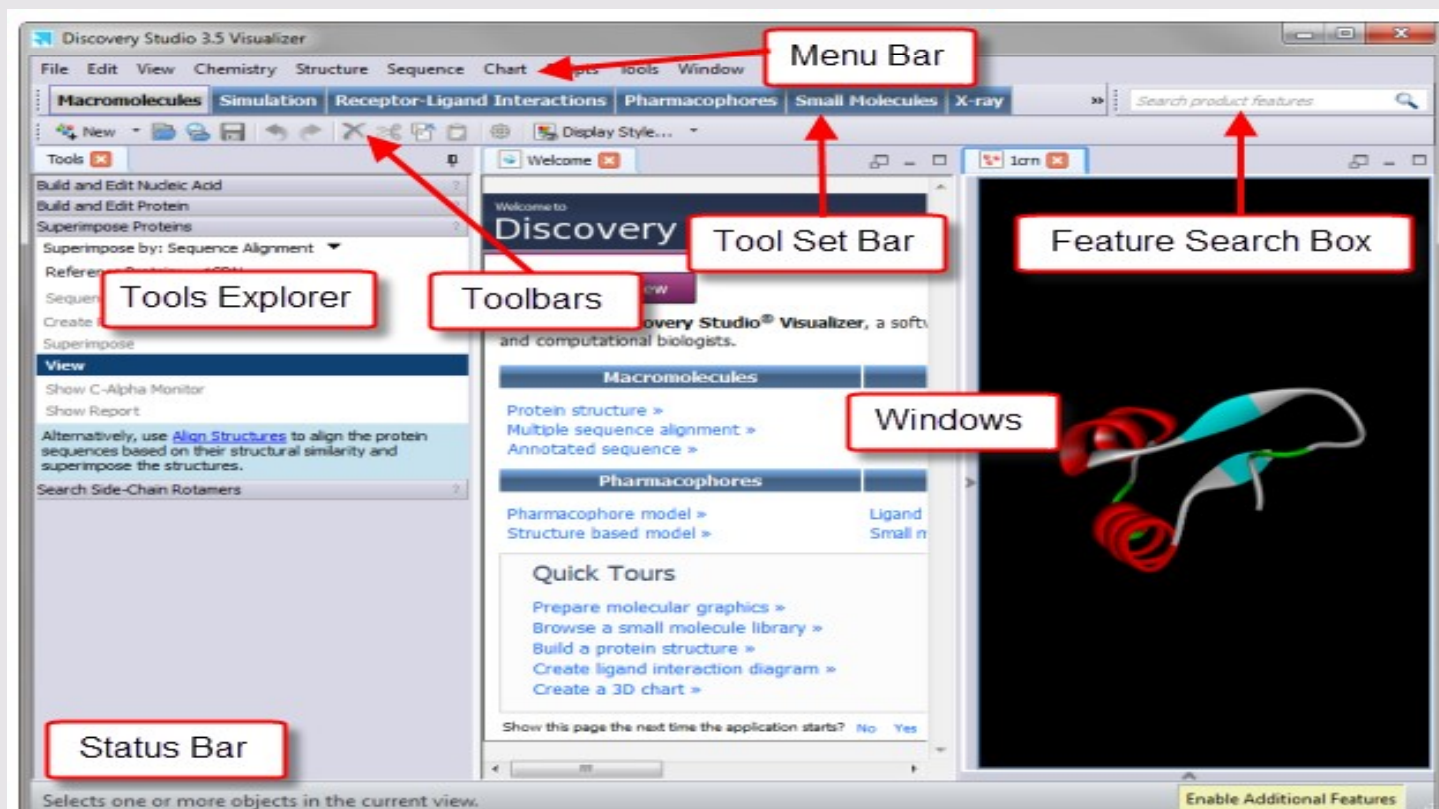




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# Application Workspace

- The application workspace occupies the main screen area when the application is opened.
- By default, a Welcome page is displayed in this space when the application is first started.
- As 2 subsequent windows are opened they can be easily arranged to either tile them or arrange them on top of each other.





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# Discovery Studio Visualizer features

FEATURE	DESCRIPTION
Feature Search Box	Use this to search and open functionality.
Menu Bar	Select menu items to access commonly used tools, such as file access, editing, and viewing commands.
Toolbars	Click buttons to gain access to commonly used tools for viewing and editing data.
Tool Set Bar	Click buttons in the tool set bar to display different groups of related analysis tools in the Tools Explorer.





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## Windows

The Discovery Studio Visualizer allows you to work with data in a variety of windows, including:

- Molecule Window: Edit and view molecular structures and property data.
- Sequence Window: Edit and view sequences and sequence alignments.
- Script Window: Create, edit, and execute Perl scripts within the Visualizer.

## Status Bar

Displays information about the current application activity.

## Files Explorer

Explore the file system to locate and open data files.



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- The application offers several ways of organizing and switching between windows.
- You can move a Window by clicking and dragging its tab to the desired position.
- In this way you can arrange windows on top of each other or organize them to view them simultaneously.

## **Tools**

- Discovery Studio offers a wide variety of tools for working with and visualizing data.
- Tools can be accessed from menus, toolbars and tool panels. In addition you can create you own tools using scripting and expose them anywhere in the application. Of all of the methods for accessing the tools, tool panels are the most flexible.



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- Tool panels group tools based on specific tasks you want to perform. Furthermore, tool panels are groups into large sets for working in areas such as Pharmacophores and Receptor-Ligand Interactions.
- A useful feature for most buttons and menu items is the tool tip.
- Hover your cursor over a feature to display a small note that offers basic information about it. In many cases, the tool tip includes a link to more detailed help or related functionality such as preferences.
- Another valuable resource for finding information about the application is the Feature Search Box in the toolbar. To locate a feature, begin typing its name, or some term that relates to its functionality.
- A list of associated features appears in a dropdown list. The Feature Search Box matches text in the short descriptions of features so matches are obtained even if you do not specify the precise name of a tool. Click on it in the list to present the corresponding menu item, toolbar button, or tool panel.