

Introduction to the Discovery Studio Client

Required functionality and modules: Discovery Studio Client.

Required data files: None.

Time: 10 minutes.

Introduction

Discovery Studio 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.

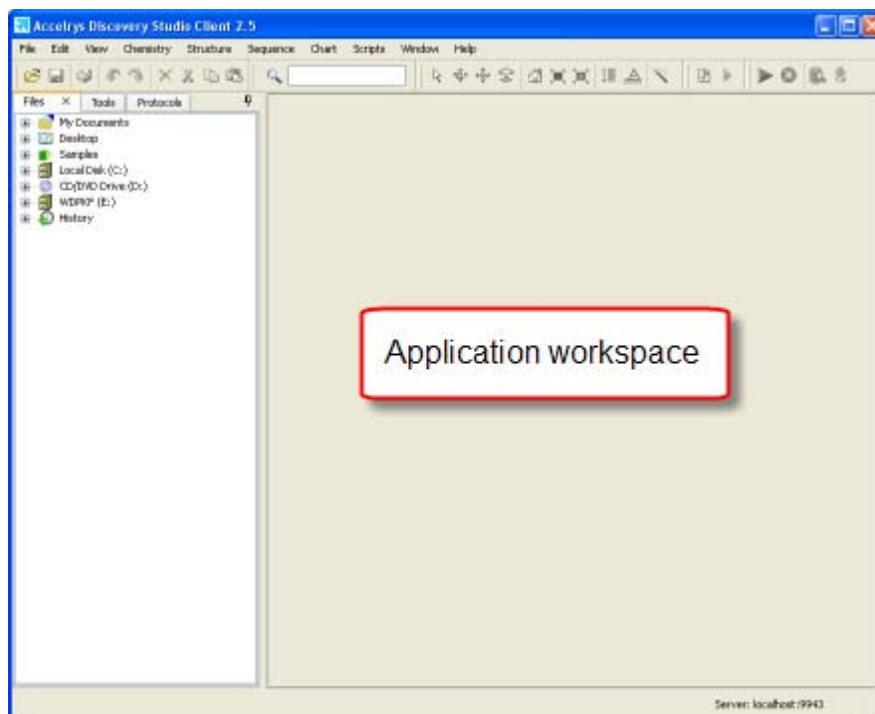
The Discovery Studio Client is a desktop application that can be used to access all the functionality in Discovery Studio. It is designed to offer an interactive environment for viewing and editing molecular structures, sequences, X-ray reflection data, scripts, and other data. It also provides a rich 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.

To get the most from the product it is useful to understand some of the key concepts and features behind the program design. This lesson provides a basic overview of how to work with the application by introducing the following basic concepts:

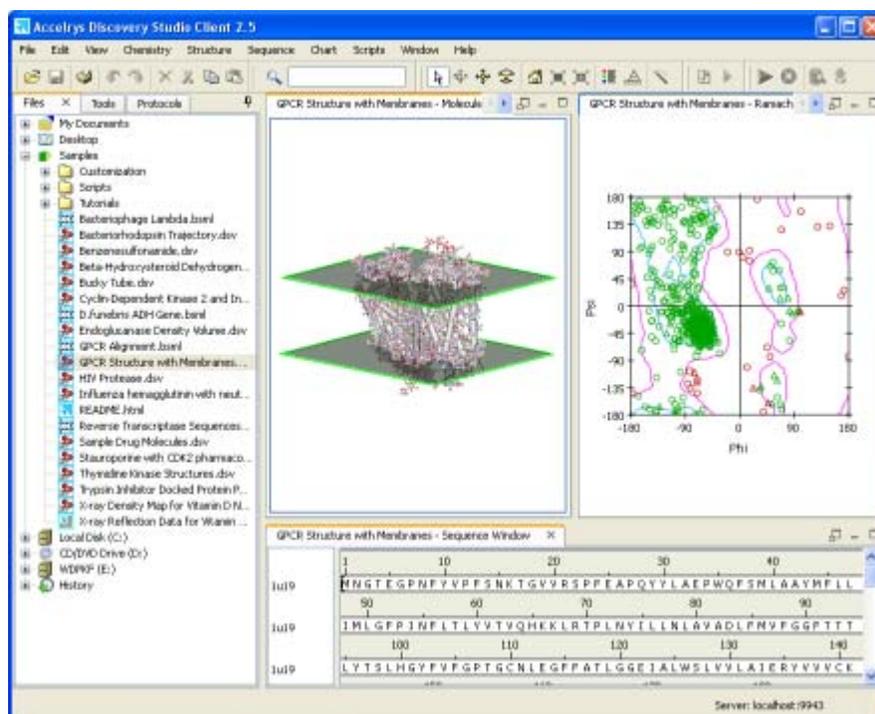
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Application Workspace

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 opened. As subsequent windows are opened they can be easily arranged to either tile them or arrange them on top of each other.

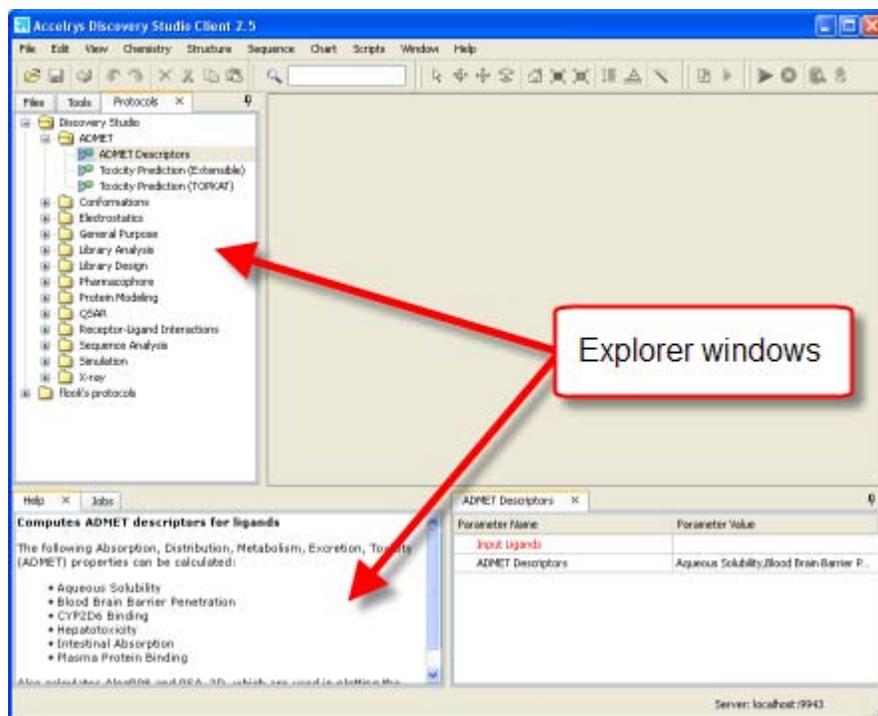


The application offers several features for organizing and switching between windows. You can move a Window by clicking dragging its tab to the desired position. In this way you can arrange windows on top of each other or organize them to view them simultaneously. You can also open windows outside of the main application window (useful when working with multiple monitors).



Explorer Windows

Explorers are specialized windows that allow you to view and access different types of data and functionality. For example, the Files Explorer allows you to view and open files. The Tools Explorer provides access to analysis tools in the application.



The explorer windows are dockable. This means that as they are dragged to different locations, they dock into those particular areas of the window. By default, several explorers dock on the left, but you could drag an explorer window to the bottom of the application workspace it will dock to the bottom of the application window. The explorer windows cannot overlap the application workspace.

It is also possible to work with explorer windows in autohide mode to increase the viewable area. To set this mode, click the pushpin at the top of an explorer dock. This causes the dock to collapse. When you subsequently click on the tab of an explorer, the window is temporarily revealed.

Note. Explorer windows cannot be dragged while they are in autohide mode.

Tools

A tool is any command that allows you to access, visualize, or analyze data. Tools can be accessed using menus, toolbars, or tool panels. In addition you can create your own tools using scripting and expose them anywhere in the application.

Protocols

Discovery Studio uses Pipeline Pilot to run complex scientific tasks. Pipeline Pilot is a data pipelining technology that makes it possible to connect different data sources with applications and rapidly process data through a branching network of computational steps. Points of data are processed independently via components, and multiple data points can be processed simultaneously via protocols.

Pipeline Pilot is tightly integrated with Discovery Studio so that data being viewed or edited in the application can be used as input to a Pipeline Pilot protocol. However, you can also edit and run protocols with the Pipeline Pilot client. You can also run Discovery Studio protocols outside of the application using other Pipeline Pilot clients such as the Pipeline Pilot WebPort.

In Discovery Studio, protocols are typically used to perform more complex multi-stage tasks, often taking significant computational time.

Note. Tools can also execute protocols. For example, a number of tools in the Tool Panel actually use fast-running protocols to perform the underlying analysis.

Menus

The main menu of the application window provides access to basic tools for accessing, editing, and viewing data. The following menus provide access to related sets of functionality:

- File

- Edit
- Menu
- View
- Chemistry
- Structure
- Sequence
- Charts
- Scripts
- Windows
- Help

Individual menu items are enabled and disabled depending on the data being viewed. The status bar provides information about what type of data is needed to enable a command, but detailed help for the tool can be opened by hovering over the tool and pressing F1.

Toolbars

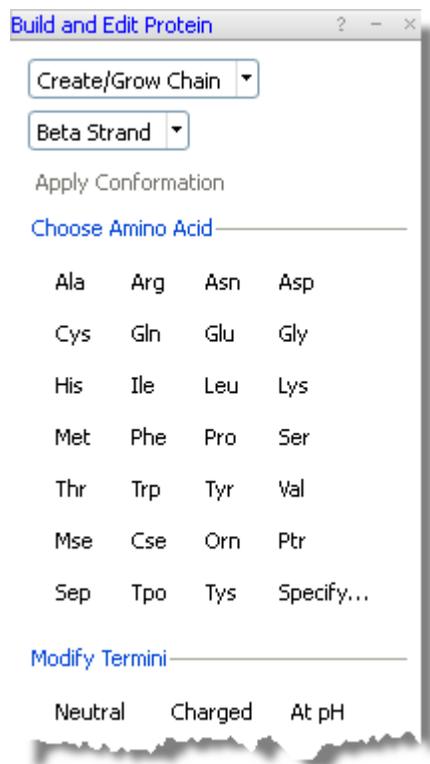
Toolbars are useful for providing easy access to commonly used, quick-running tools. A large set of toolbars are provided, which can be shown or hidden depending on the current task. By default, a set of general purpose toolbars such as Standard and Display are shown when you start the application for the first time. However, as you start to work with the application you can add additional toolbars by right clicking on an existing toolbar and selecting from a drop down list.



Tool Panels

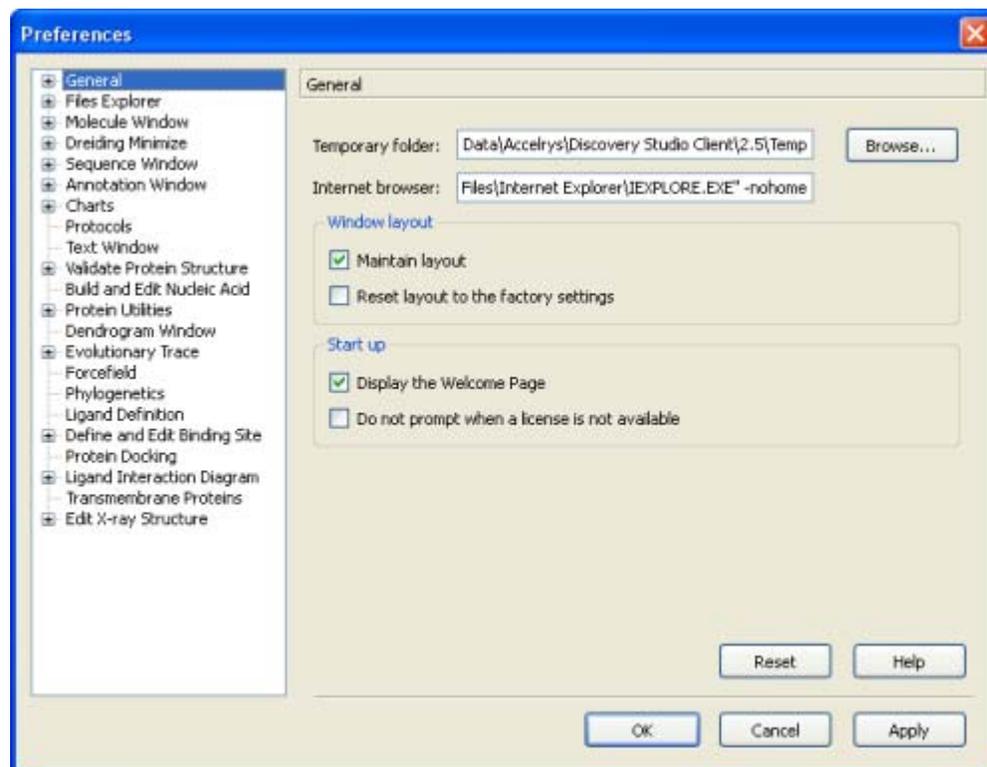
Tool panels are another way of invoking tools to analyze data. Tool panels are graphical palettes that contain buttons, dropdowns and other controls that provide access to related sets of functionality. The tools exposed on tool panels typically operate directly on a selected object in the current window, and like other tools, are enabled and disabled depending on whether the appropriate data is selected.

Tool Panels are located in the Tools Explorer. You can view related sets of tool panels by using the drop down control at the top of the Tools Explorer to select a particular set (e.g. Visualization, Sequence Analysis) or create your own sets of tool panels that combine commonly used tools. Custom tool panels can be created from the Tools Explorer or using the Tool Panels preferences page.



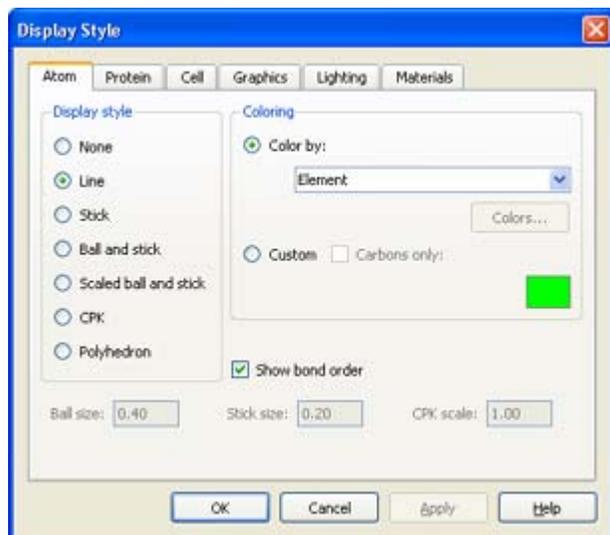
Preferences

Application customization and settings are available in the Preferences dialog, which can be accessed from the Edit menu. The dialog contains a tree control that lists the different preferences categories. By clicking on the area of interest, the main preference page displays the available options.



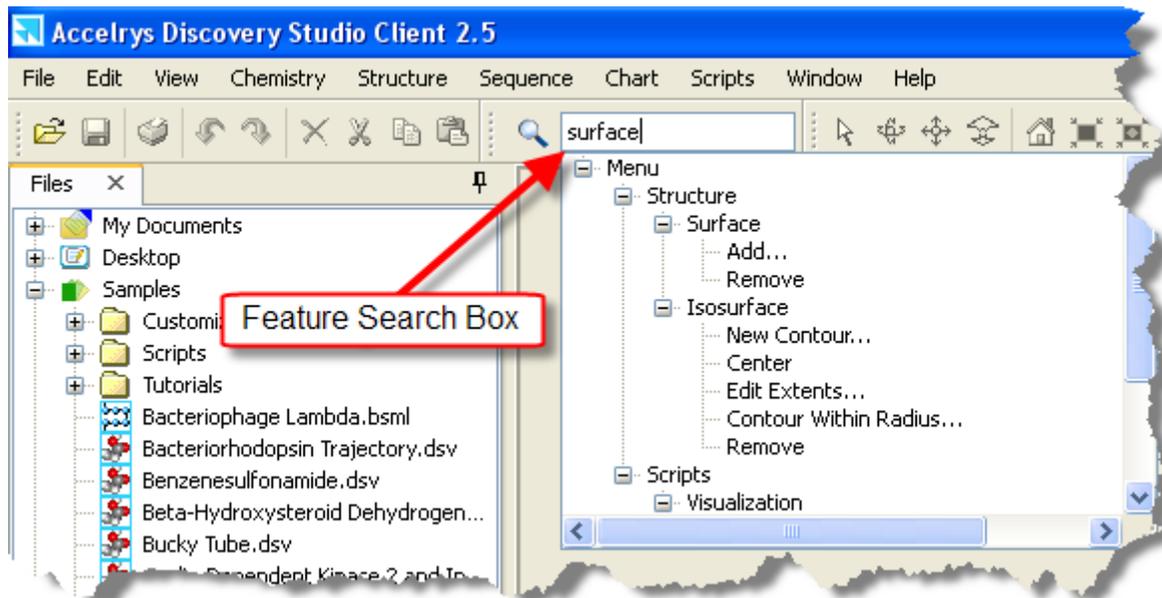
Display Style Dialog

While the Preferences dialog provides access to application-wide settings, the Display Style dialog is used to change the settings that affect the appearance and behavior of specific data opened in different windows. When data is opened in the application, you can access this dialog by right-clicking the view or from the View menu. This dialog provides access to settings that control particular aspects of the appearance of data or the way the display is configured. Any changes made in the display style dialog are stored with the data if it is saved in a Discovery Studio file format (.dsv).



Feature Search Box

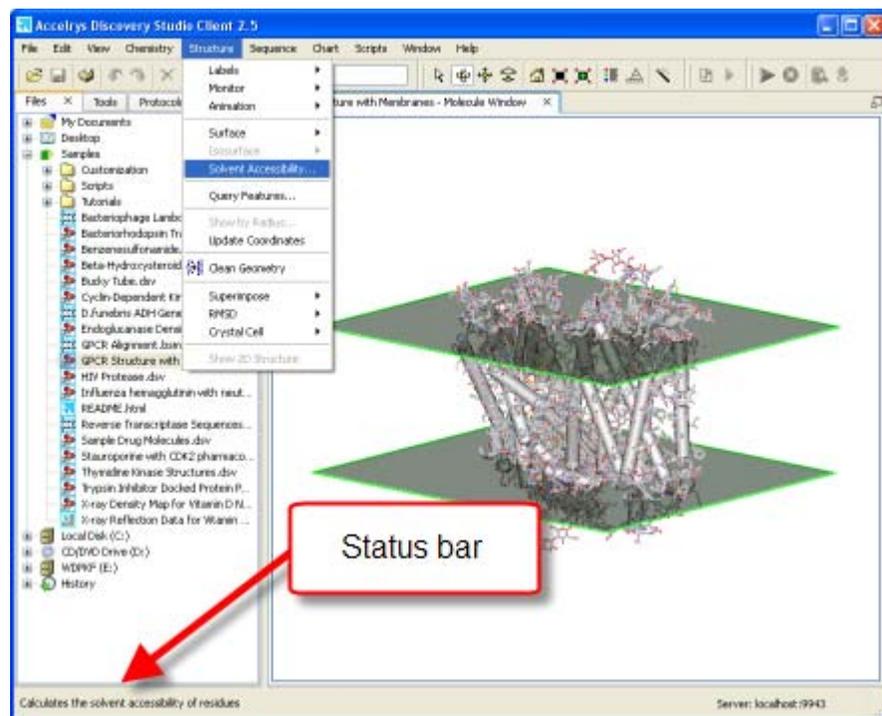
The Feature Search Box in the toolbar is a valuable resource for finding and navigating to functionality in the application. To locate a feature, begin typing the name of that feature, or some term that relates to its functionality. A list of associated features appears in a dropdown list. The Feature 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, tool panel or protocol.



Status Bar

The Status Bar at the bottom of the application window displays information about the current activity. It is particularly useful when selecting menu items, toolbar buttons, or tool panel items as it displays information about

how to use that feature. In addition, when working with molecules or sequences, the Status Bar often displays information about the state of the selected object.



Scripts

Discovery Studio provides a Perl Application Programming Interface (API) to allow development of custom scripts. This powerful feature enables the creation of Perl scripts that automate commonly used tasks in the application. In addition, because the API provides full access to the underlying data models in the application (e.g. the Molecular Data Model, the Sequence Data Model), you can create scripts that perform advanced analysis routines if desired.

Another powerful feature of scripting in the Discovery Studio Client is that the API provides functions for accessing data already in memory. This enables the creation of scripts that process molecules, sequences, or other data that you happen to be editing. In this way it is possible to create new tools that can be invoked through menus, toolbars, or tool panels. For details, see [Working with scripts](#).