

Viewing ligands in a 2D window

Required functionality and modules: Discovery Studio Client

Required data files: 1aq1.pdb

Time: 10 minutes

Introduction

The 2D Window can provide a flattened graphical view of small molecules within a receptor. This tutorial introduces the basic features of the 2D Window and the creation of a flattened depiction of the ligand-receptor interactions. The following tasks are covered:

- [Identifying ligands](#)
- [Generating the ligand-receptor interaction view](#)

Identifying ligands

Before generating a 2D depiction of the ligand-receptor interactions, it is necessary to identify the ligand. The diagram allows for a broad definition. A ligand may consist of one of the following:

- single chain of residues in a molecule
- several residues within a chain (a subset of a chain)

In all cases, the maximum number of atoms allowed is 1000.

In addition, the ligand consists of a single connected entity or fragment. Bonds from the ligand to the receptor are allowed. For the purposes of the diagram, the receptor (or external environment) consists of all unselected atoms.

Several commands on the Analyze Binding Site tool panel are provided to assist in identifying ligands. The command Create Ligand Groups will identify any molecule or chain that can be considered a ligand. The maximum number of atoms for automatic identification is 200.

From the **Files Explorer**, open **Samples | Tutorials | Receptor-Ligand Interactions | 1aq1.pdb**.

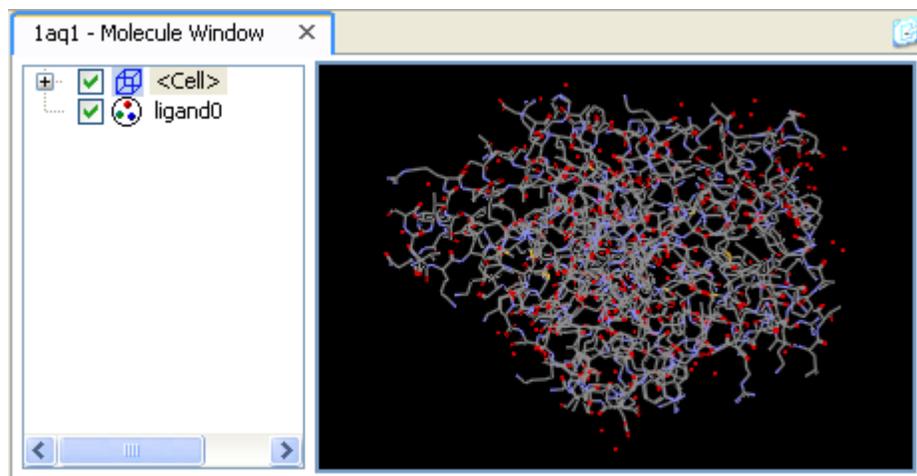
If the Hierarchy View is not displayed, choose **View | Hierarchy** from the menu bar.

Open the **Tools Explorer**.

If the Analyze Binding Sites tool panel is not available, choose **View | Tool Panels | Analyze Binding Sites** from the menu.

Click **Create Ligand Groups**.

The contents of the file is displayed in a Molecule view and a new **Group** named `ligand0` has been added to the **Hierarchy View**.



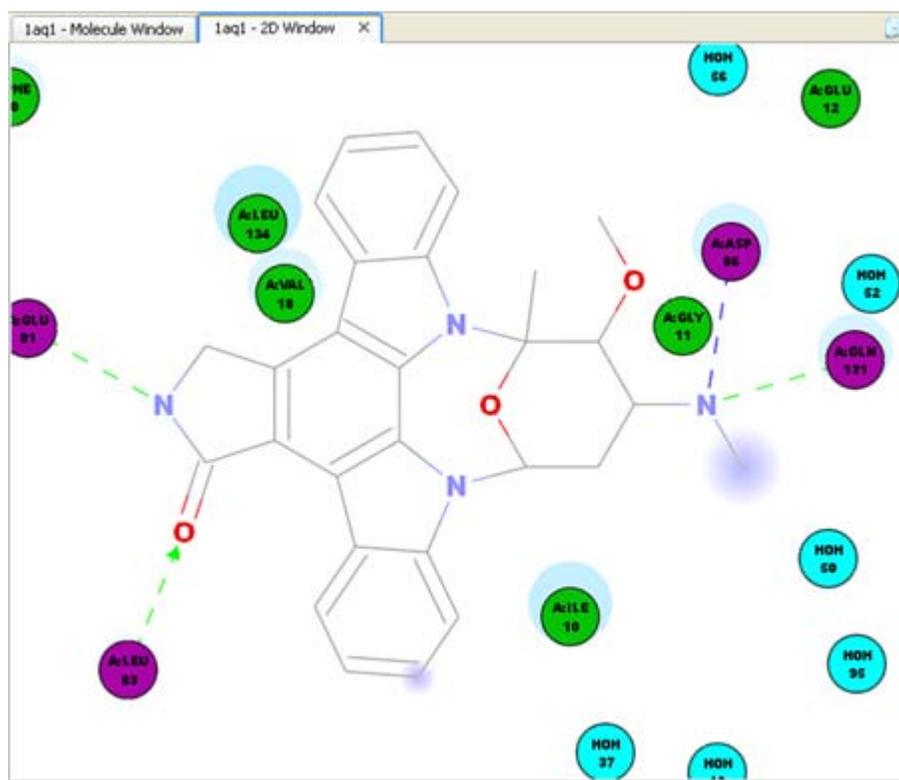
Generating the ligand-receptor interaction view

With the ligand identified, you can now generate the ligand-receptor interaction view.

From the same tool panel, click **Select Ligand Group**.

Click **Create Ligand Interaction View**.

After a few seconds, the 2D Window will open. The ligand is flattened to two dimensions. Interacting residues are displayed as colored discs. H-bond, charge-charge, and Pi-bond interactions are displayed as dashed lines. The solvent accessible surface is shown as a diffuse background circle with the radius proportional to the exposure. Many options are available in the Display Style dialog to customize the appearance.



You can now analyze the ligand-receptor interactions from both the 2D and 3D Molecule Windows. To help compare views, zoom in on the ligand-receptor on the Molecule Windows.

With the **2D Window** active, press **CTRL+A** to select all 2D objects.

Activate the **Molecule Window**.

From the menu bar, choose **View | Transform | Fit To Screen**.

The ligand-receptor binding site is now centered in both windows. For large ligands, the 2D depiction of the ligand can be slow. To improve the response time, you can modify the *Ligand quality* option in the [Ligand Interaction Diagram page - Preferences dialog](#). Set the value to **Medium** or **Low** to improve the response time.

Further information

[Receptor Ligand Interactions](#)