

## Preparing a receptor binding site

**Required functionality and modules:** Discovery Studio Client.

**Required data files:** 1kim.pdb.

**Time:** 10 minutes.

### Introduction

The receptor binding site is important for docking and scoring applications. It defines a region in a protein cavity where binding interactions can occur.

For most protocols, a sub-section of the binding site is defined by a sphere that encloses part of the binding site volume.

In this tutorial, you will learn how to find binding sites and define a search sphere. This tutorial covers:

- [Finding a Binding Site from receptor cavities](#)
- [Define a Binding Site Sphere from a Binding Site Cavity](#)

### Finding a Binding Site from receptor cavities

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

The protein opens in a new Molecule Window.

At the top of the **Tools Explorer**, select the **Receptor-Ligand Interactions** layout from the list.

This opens the Receptor-Ligand Interactions tool panel layout.

Select any protein atom in the Molecule Window.

From the **Define and Edit Binding Site** tools group, under **Define**, click **Define Selected Molecule as Receptor**.

This defines the receptor molecule as a receptor. You can now run the site finding algorithm.

From the Tools Explorer, under **Define and Edit Binding Site** tools group, click **Find Sites from Receptor Cavities**.

Green grid points now show the location of the first receptor binding site.

You can view the other binding sites by repeatedly clicking **Next Site** from the **Define and Edit Binding Site** tools group.

### Define a Binding Site Sphere from a Binding Site Cavity

Now you will define a site sphere from a binding site cavity.

In the **Hierarchy View**, expand **<Cell>**, then expand **1kim**. If the Hierarchy View is not visible, press **Ctrl+H**.

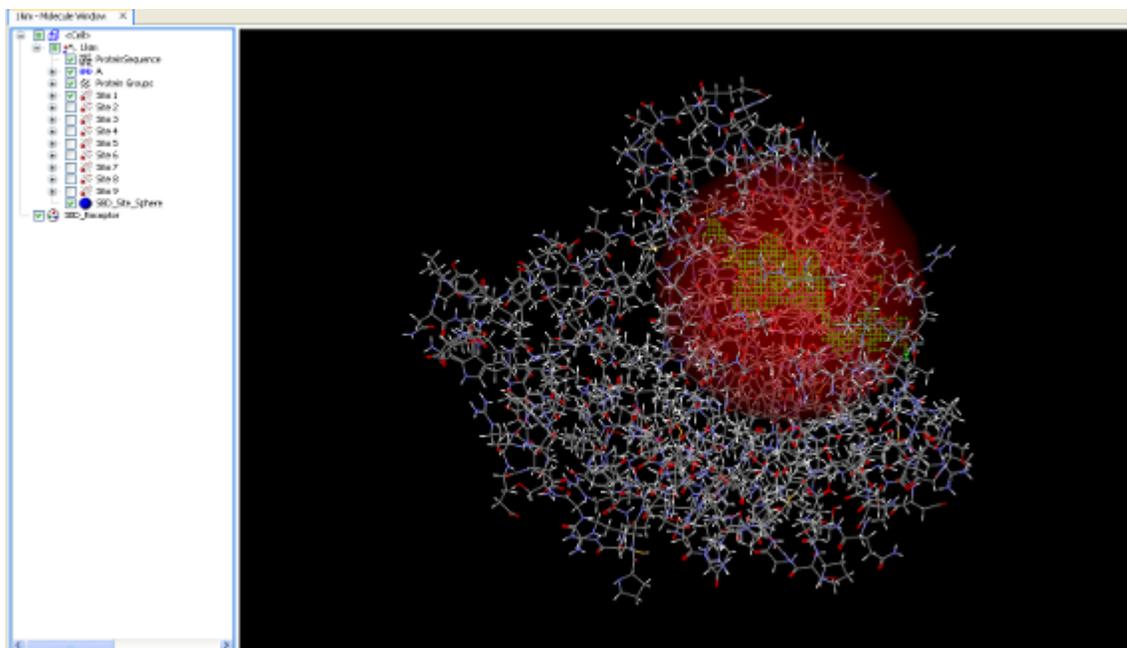
Notice that there are nine binding sites.

Select **Site 1** (make sure the site is visible).

Notice that the site points turn yellow when they are selected.

From the **Define and Edit Binding Site** tools group click **Define Sphere from Selection**.

A red sphere now encloses the binding site points:



**Note.** Any atom selection can be used for define the center of the binding site sphere. Additionally, the radius of the search sphere and the size of the binding sites can be increased and decreased from the tools panel with the **Contract Binding Sites/Spheres** and **Expand Binding Sites/Spheres** tools.

### Further information

[Receptor-Ligand Interactions](#)

[Define binding site and site partition](#)