User Manual

Running the program

At the command line while in the rdock_gui directory type java gui.Main_gui and the GUI should appear. Please in any file names and directories do not have spaces.

Using the program

Resizing the GUI

You can resize the graphical user interface (GUI) by dragging it from the sides and corners like most other applications. If you make it smaller than the minimum size to fit all the items in, scrollbars will appear in the appropriate place – i.e. along the bottom, along the right hand side or both. (See fig1) You can get tooltips by hovering over buttons and certain other areas of the GUI – these give you more information than is shown on the button about what the button does. (See fig 1)

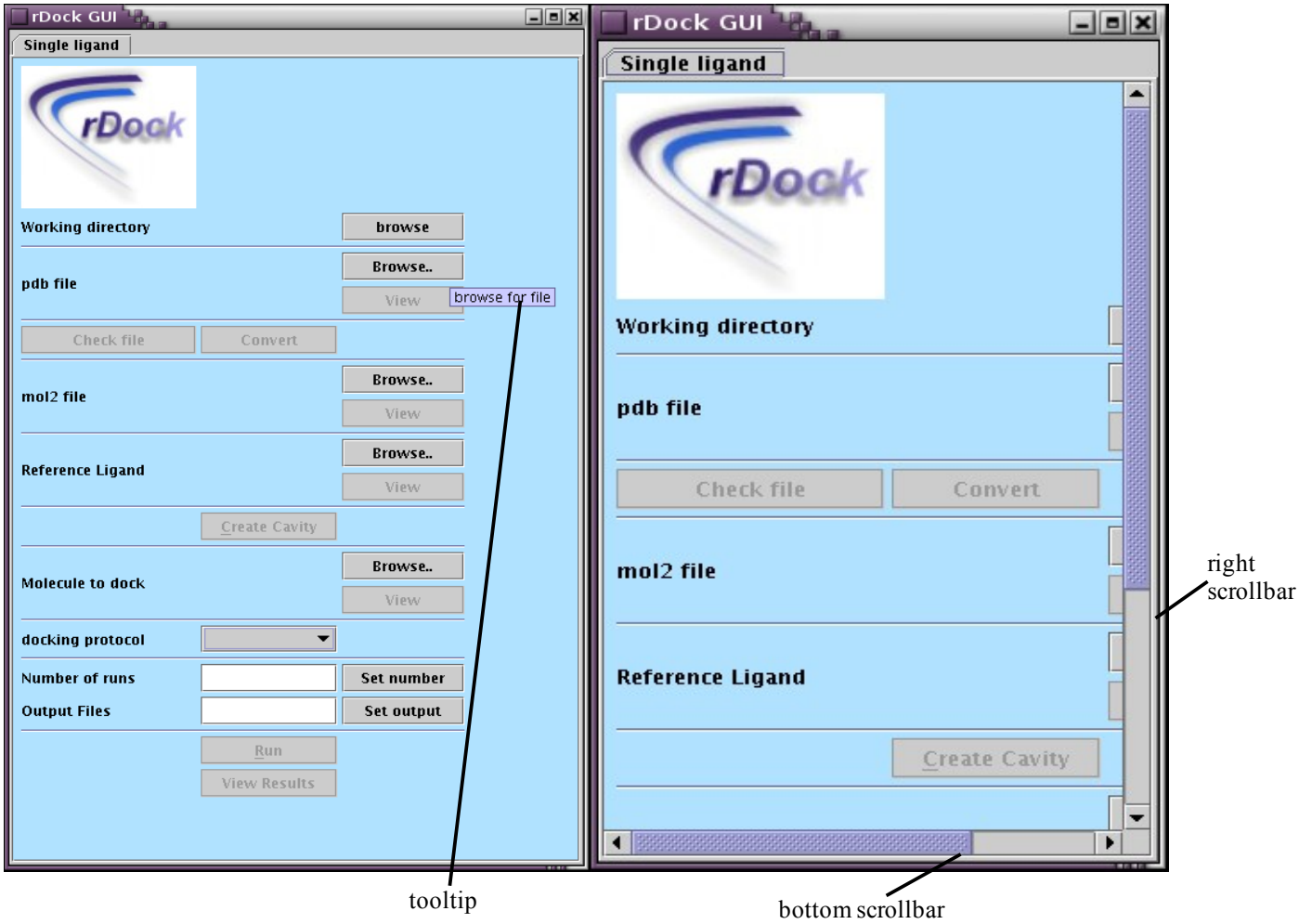

Fig 1 The left hand image shows the GUI at its full size when it is first loaded. If you resize it so that it becomes smaller and as such not all of the items fit in scrollbars will appear as appropriate – on the bottom, on the right or on both. These can be used to access unseen buttons. Also shown is a tooltip – these appear when you hover over buttons and other parts of the GUI.

Setting your working directory

In order for files to appear in an appropriate location you need to set your initial working directory. To do this select the browse button under the working directory area. (See figure 2) The directory will appear in this area and can be changed as required by pressing the browse button and selecting a different directory. When you press the browse button you will be presented with a file chooser dialogue where you can select your required directory. (See fig3)

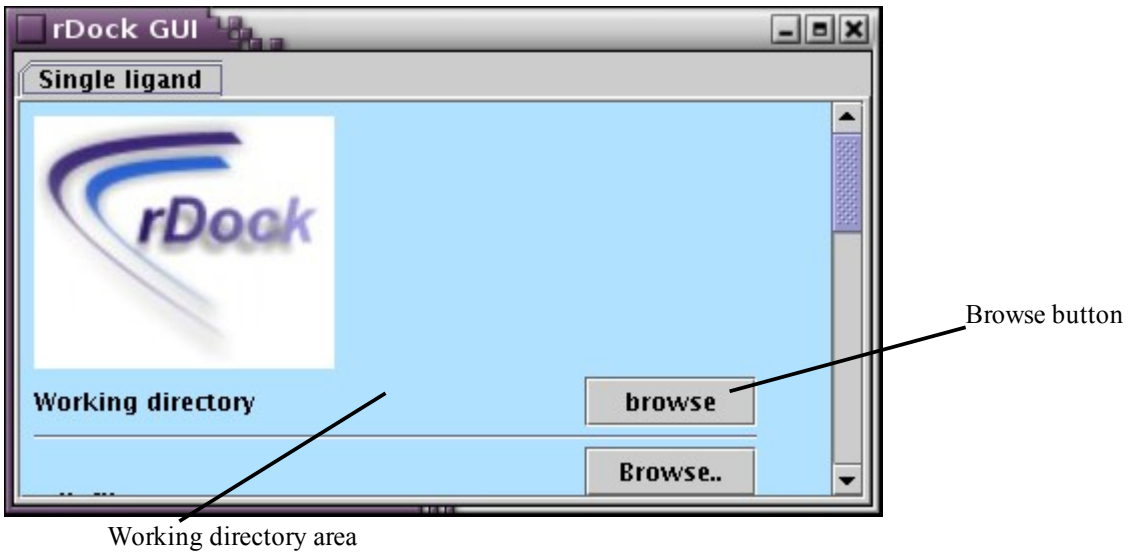

Fig2 Top section of GUI showing the working directory area and the browse button for the working directory.

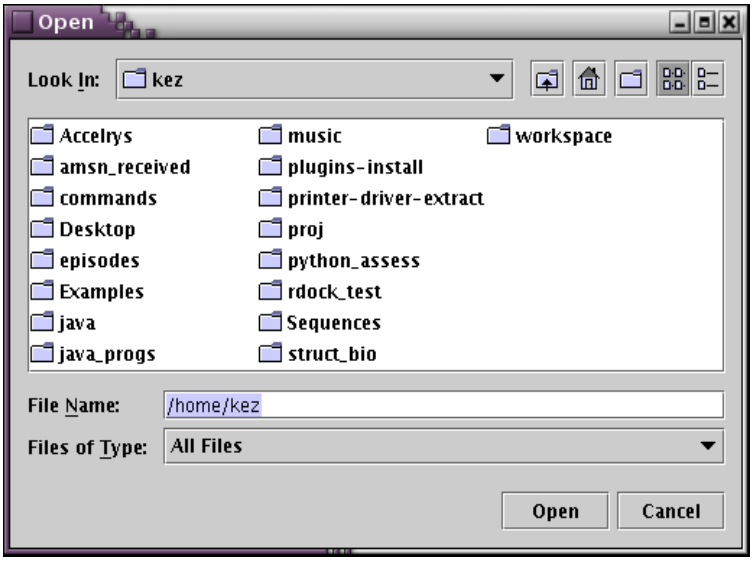

Fig3 File Chooser dialogue so you can choose directories and files as appropriate

What next?

Now you need to work out which case applies to you. Either you will have a pdb file that you wish to check and then convert to a mol2 file or you will already have a mol2 file, in which case you don't need to bother with the pdb file.

I have a pdb file

If you are starting with a pdb file you should browse for the file using the browse button contained within the pdb file area. (See fig4) The file you choose will be displayed within the area. Once you have chosen an appropriate file you can view it in DSVisualizer which you can do by pressing the view button (see fig4) and then you can edit and then save the file – if you make any changes to the file that you wish to use for docking you can either save it as the same file and you don't need to change anything but if you save it as something else and wish to use you new version you must re-choose your new file using the browse button. Before you convert the file you should check it for errors by pressing the check file button (see fig4) – a text file will be produced called Errors.txt – it will appear automatically and will inform you of any errors – if there are none you can proceed but if there are some the errors should be dealt with and the file rechecked before conversion or the conversion wont work. Once you have a pdb file that is free from errors you can convert it to a mol2 file by pressing the convert button (see fig4).

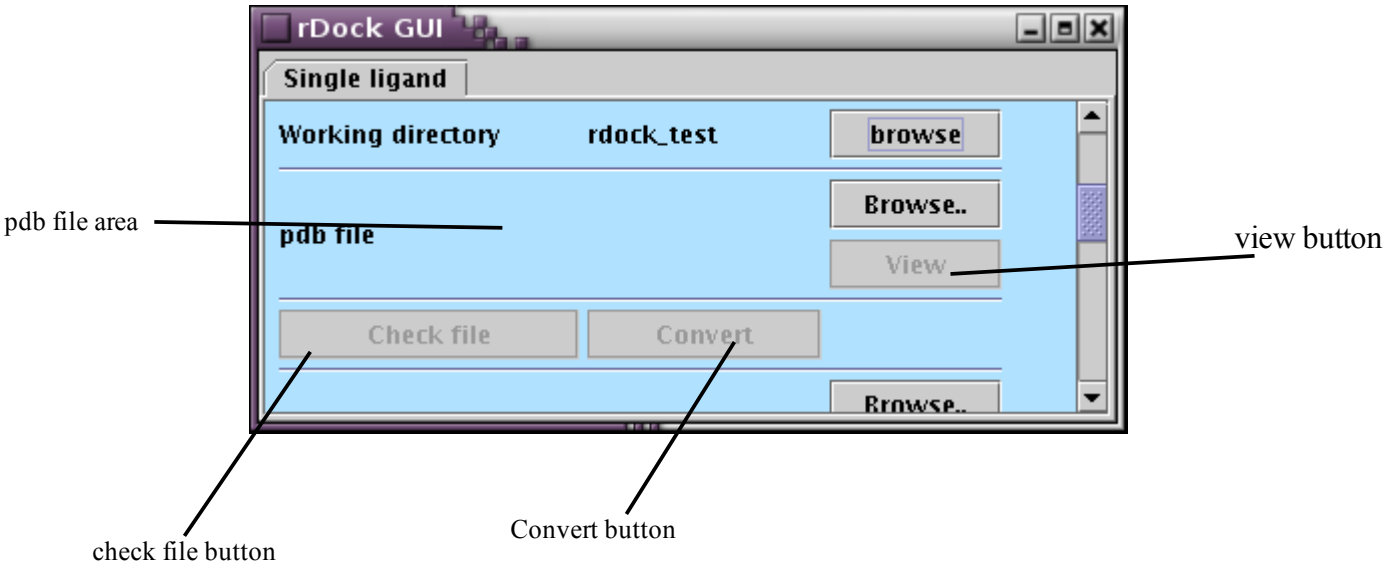

Fig4 Section of the GUI that shows the pdb file area with its browse and view buttons In the area below can be seen the check file and convert buttons.

Selecting a mol2 file

To select a mol2 file use the browse button within the mol2 file section to find either an existing mol2 file or the one you just created by using the convert button.

Selecting a reference ligand

This will be a .sd file and can be selected using the browse button in the reference ligand section. Again it can be viewed by using the view button in its section.

Creating a cavity

Once you have a mol2 file and a reference ligand you will be able to create a cavity by clicking on the create cavity button, which will have become activated (see fig5) this might take some time to do. Pressing this button will create a .prm file and will run the rbcavity program which produces a .as file.

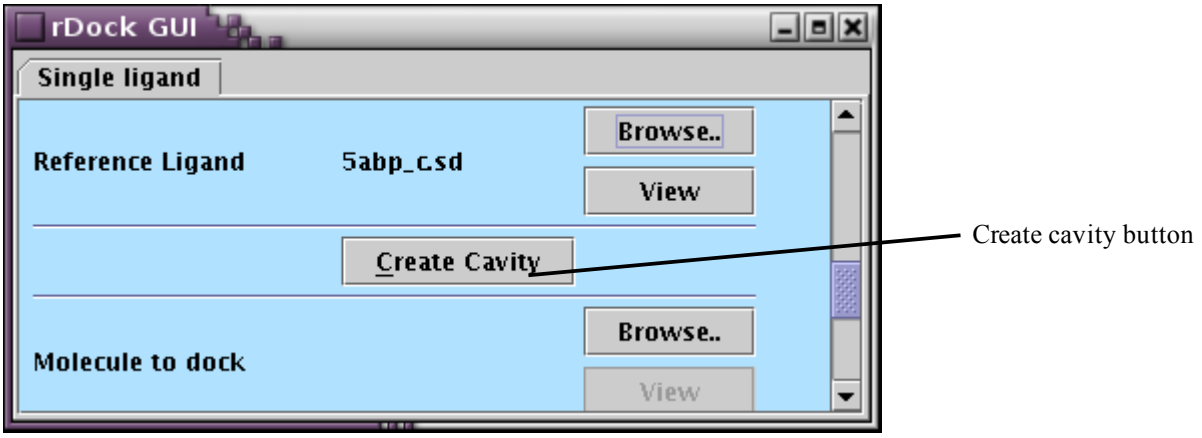

Fig5 Section of the GUI displaying the create cavity button

Selecting the molecule to dock

To select the molecule that you wish to dock with your protein use the browse button in the molecule to dock section. Once you have selected it you canview it using the view button contained within that section.

Selecting a docking protocol

Select the docking protocol that you wish to use from the drop down menu that is in the docking protocol section (see fig6). To select an option click on the arrow (See fig 6) and the click on your choice.

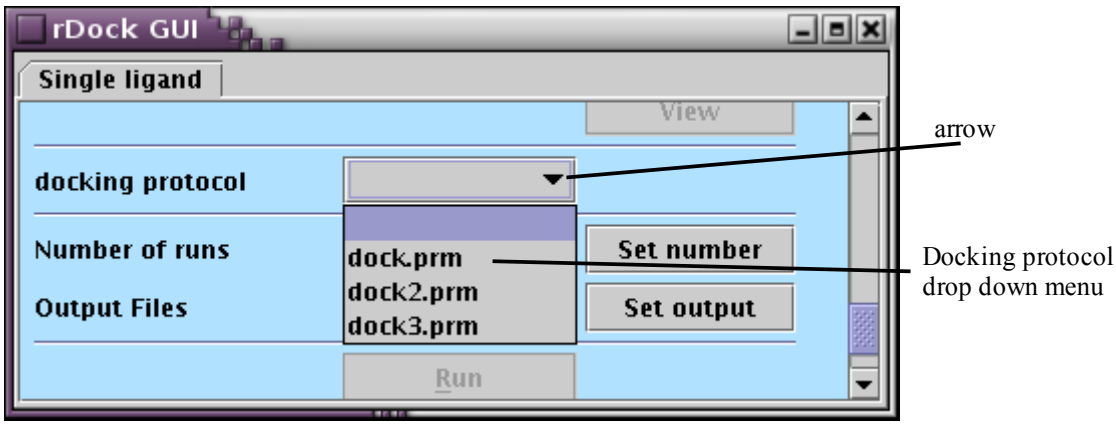

Fig6 Docking protocol section showing the docking protocol drop down menu and the arrow that provides you with the list

Entering the number of runs

Type the number of runs that you wish to carry out into the box in the number of runs section and either press enter or use the set button (See fig7)

Entering your output file

In the box in the output file section type in the name of your desired output file – this will be located in your working directory. After entering it you should either press enter or the set button. (See fig7)

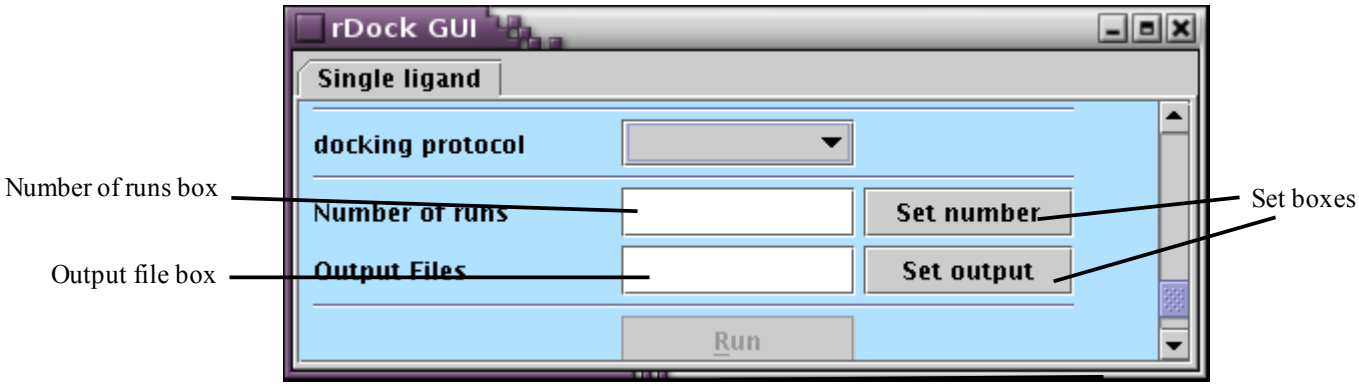

Fig7 Section of the GUI showing the number of runs and output files boxes as well as the set boxes.

Running rDock

Once you have filled in all the required information the run button will become enabled (See fig8). If you press it rDock will run and output files will be generated in your working directory. You can view these results by pressing the view results button below the run button (see fig8).

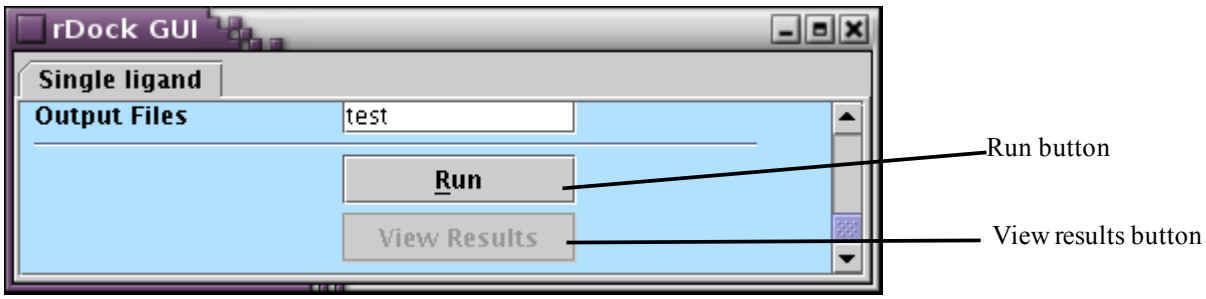

Fig8 Section of the showing the run button and the view results button.