Instillation Guide

Required other programs

You must have rDock installed and the appropriate path variables set up for it (see the rDock documentation).

You must also have java installed on your machine so you can actually run the GUI.

Babel should also be installed and the path set up for it – this is only necessary if you are going to use the GUI to convert pdb files - you can also create a mol2 file by saving a pdb as mol2 in DSVisualizer.

To use the view functionality DSVisualizer should be installed.

Installing the GUI

Unzip or untar the folder called rdock_gui.zip or rdock_gui.tar. This should give you an outer folder called rdock_gui with an inner folder called gui. In the outer folder you'll find a template file called path_template.txt which contains two lines – one starting GUI: and the other starting Protocols:. After GUI: you should type the full path of where the script Completeeerrors.pyc, and rdock2.jpg – these should at the moment be in the same folder as the template that your editing but they don't have to be as long as they are all in the same folder and path_template.txt doesn't get moved as well. After Protocols: you should type the full path of where all your docking protocols are – they should be in their own folder that has no sub folders. Please save this folder and don't move it from this location – you can move the other documents in this directory – as long as you change it in the template, but you cant move the subdirectory gui. All paths should have no spaces in them.