

Virus mutation and docking simulation

Installation Guide

Install AutoDockTools

AutoDockTools is a cross-platform, GUI front-end for AutoDock. This provides an easy-to-use interface for setting up docking simulations and running them.

Install AutoDockTools on Windows

The Windows version of AutoDockTools is included in the MGLTools package and can be downloaded from [the official download site](http://mgltools.scripps.edu/downloads) (<http://mgltools.scripps.edu/downloads>). The latest version is 1.5.6. Choose the “mgltools.win32.1.5.6_Setup.exe” for the simplest installation. After downloading, simply follow the on screen instructions to install the software. Installation requires an administrator password.

Install AutoDockTools on Mac OS X

The Mac version of AutoDockTools requires XQuartz, a free and open-source version of the X.Org X Window System for OS X. You should check to see if you already have XQuartz installed. To do this, click “Go → Utilities” in your menu bar. A Finder window will open. If you see “XQuartz” in this Finder window, you already have it installed. If instead you see “X11,” you do not. You can download and install XQuartz by double clicking the “X11” application in the Utilities folder and following the on screen instructions. Alternatively, you can download XQuartz at the official website, www.xquartz.org (www.xquartz.org). The package installer will require an administrator password.

Following installation, you can install the latest version of the MGLTools package (which contains AutoDockTools) from [the official download site](http://mgltools.scripps.edu/downloads) (<http://mgltools.scripps.edu/downloads>). The most recent release is MGLTools version 1.5.6. For the easiest installation, download the Mac installer on the left side of the table, “(Snow) Leopard - Mac OS X 10.5 and 10.6 - Intel.” Open the disk image and double click on the package installer. Again, installation requires an administrator password.

Install AutoGrid and AutoDock

AutoGrid and AutoDock are responsible for making the files necessary to run and running docking simulations, respectively. They are separate from AutoDockTools and are command line based applications. Download the version appropriate for your computer from the [the AutoDock download page](http://autodock.scripps.edu/downloads/autodock-registration/autodock-4-2-download-page) (<http://autodock.scripps.edu/downloads/autodock-registration/autodock-4-2-download-page>).

Install AutoGrid and AutoDock on Windows

The download from the website is again an installer program. Follow the on screen instructions and enter an administrator password to install the software in the default location.

Install AutoGrid and AutoDock on Mac OS X

The download from the website is a tarball containing the two executables. After downloading, double click the tarball to extract it. Inside you will see two files, `autodock4` and `autogrid4`. You can place these files anywhere on your system, so long as you remember where they are located.