Required software

# Chimera

## Windows

1. Download the Windows installer from (see picture below): <https://www.cgl.ucsf.edu/chimera/download.html>
2. Run the installer (standard options should suffice)
3. Make sure shortcuts were made (e.g. in Start-menu or on Desktop)

## MacOS

1. Download the .dmg file from (see picture below):  
   <https://www.cgl.ucsf.edu/chimera/download.html>
2. Open the .dmg and drag Chimera to the Application folder
3. Chimera shortcut should now be available in your Application browser

Afbeelding met tekst, schermopname, Lettertype, nummer

Door AI gegenereerde inhoud is mogelijk onjuist.

# LigPlot+

## Windows + MacOS

1. Download the LigPlus folder from the following link:  
   <https://www.dropbox.com/scl/fo/fxqvdq1755a5m42opwtsn/AFc7nZgfqmB3HwVjDXj79Ls?rlkey=lkzvlip1v6cqm6w2ramovrbv8&dl=0>
2. In the downloaded folder you will find “LigPlus.jar”
   * Typically your system will already have a java install, you can then simply double click to open LigPlot+
   * If your system does not have a java environment installed, please find a suitable version from: <https://www.java.com/en/download/manual.jsp> and install it
3. The first time you open “LigPlus.jar” the program will ask for some information. The standard options are fine, but make sure the “Temporary Directory” is set to a folder on your system: Afbeelding met tekst, schermopname, lijn, Lettertype

   Door AI gegenereerde inhoud is mogelijk onjuist.

Afbeelding met tekst, schermopname, nummer, Lettertype

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# AutoDock Vina (optional)

## Windows

1. Download the Windows executable “**vina\_1.2.7\_win.exe**” from (see screenshot at the end):   
   <https://github.com/ccsb-scripps/AutoDock-Vina/releases/tag/v1.2.7>
2. Make sure the file is somewhere on your system where you can easily find it

## MacOS

Please note: getting Autodock Vina running on MacOS is a bit difficult and if you experience problems with the instructions, please feel free to reach out to Charles-Alexandre.

1. The correct executable will depend on your system (see screenshot at the end):
   * Intel chipset (older Macbooks): “**vina\_1.2.7\_mac\_x86\_64**”
   * Apple chipset (newer Macbooks): “**vina\_1.2.7\_mac\_aarch64**”

Download the correct executable from   
<https://github.com/ccsb-scripps/AutoDock-Vina/releases/tag/v1.2.7>

1. Make sure the file is somewhere on your system where you can easily find it
2. MacOS is very strict towards 3rd party applications. We need to explicitly allow the execution of the vina\_1.2.7 executable:
   * Open a command line terminal and navigate to the folder where you placed the vina\_1.2.7 executable:  
     $ cd /path/to/file
   * Change permission of the file to allow execution:  
     $ chmod +x vina\_1.2.7\_mac\_aarch64  
     or  
     $ chmod +x vina\_1.2.7\_mac\_x86\_64
   * Try to execute vina:  
     $ ./vina\_1.2.7\_mac\_aarch64  
     or   
     $ ./vina\_1.2.7\_mac\_x86\_64
   * MacOS will now warn you about the developer not being trusted and will not execute vina
   * Open “System Settings” and navigate to “Privacy & Security”
   * Scroll down and you should find a similar message:  
     A screenshot of a computer

     AI-generated content may be incorrect.
   * Click “Allow Anyway” and confirm with your password
   * If you go back to the command line and try to run vina again, it should now work. (You might get an additional warning but you should be able to click “Open” and it you should see some output.)

Afbeelding met tekst, schermopname, software, nummer

Door AI gegenereerde inhoud is mogelijk onjuist.