

Installing NMRPipe on your computer

Macro Methods

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This quick guide will help with installation of the NMRPipe software, which was created by Frank Delaglio at the NIH/NIST. It is a powerful program for processing high-dimension biomolecular NMR data and can be used to process data from Bruker, Varian, and JEOL instruments. We'll be using it to process the HSQC data we get in the second week of the course.

Setup for Mac and Linux systems can be found at <https://www.ibbr.umd.edu/nmrpipe/install.html>, which is also posted on the class website. I've pared down the information from this site and provided information specifically for newer versions of Mac OS. If you need to install on Linux or older systems, the website is a good place for assistance and troubleshooting.

Part I: Change Default Shell and set up directory

1. Open either XQuartz or the Mac terminal from the Applications/Utilities/ folder
2. Type 'chsh -s /bin/tcsh' (no quotes) to change the default shell to C-shell, which is required to run the NMRPipe software. You can always set the shell back to bash (or whichever you choose) by typing 'chsh -s /bin/bash'.
3. Navigate to your home directory by typing 'cd ~'. Type 'ls' and you should see familiar folders like Documents, Downloads, etc.
4. Make a directory for NMR-related files: 'mkdir nmr'

Part II: Install NMRPipe

1. Navigate into the newly created nmr directory: cd nmr/
2. Use the curl command to download the following:

```
curl -O https://www.ibbr.umd.edu/nmrpipe/install.com
curl -O https://www.ibbr.umd.edu/nmrpipe/binval.com
curl -O https://www.ibbr.umd.edu/nmrpipe/NMRPipeX.tZ
curl -O https://www.ibbr.umd.edu/nmrpipe/s.tZ
```
3. Make the appropriate changes so the files can be read and executed:

```
chmod a+r *.tZ *.Z *.tar
chmod a+rx *.com
```
4. Run the install file: ./install.com

If things go as planned, the installation should be finished and NMRPipe is ready to go! To test this, you can type 'nmrPipe' in the command line and press enter. The version installed should appear. You can also try 'bruker' and a GUI will open, which we will use later.

In the case there is an error, it is likely because you need to add two if-statements to the terminal .cshrc file that is run each time you initiate a session with terminal/XQuartz. To do this, edit the .cshrc file by typing 'nano .cshrc' and add the following to the end of the file (change the highlighted part of the path to reflect the actual location of your nmr directory):

```
if (-e /Users/student/nmr/com/nmrInit.mac11_64.com) then
    source /Users/student/nmr/com/nmrInit.mac11_64.com
endif

if (-e /Users/student/nmr/com/font.com) then
    source /Users/student/nmr/com/font.com
endif
```

Save the file by typing 'control+X' and 'Y'. Every time you edit this file you need to logout of the computer for the changes to take effect. Try running NMRPipe again and hopefully this time it will work properly.