Saving, Transferring and Processing NMR Data

Saving NMR Data on the Inova after Completion of Data Acquisition

1. At the conclusion of any nD data acquisition, be sure to save your data to the designated directory. This directory is typically named after you (last and/or first name) under the directory `/space2/home/ishwar/data`. You could either navigate through the Vnmr menus to get there or just type within Vnmr: `cd ('/space2/home/ishwar/data/yourname')`
2. Create an appropriate subdirectory under this directory for this sample (e.g. 15N13C_SF1DBD+SBS_H2O).
3. Give a descriptive filename and save your data using the `svf('filename')` (no space between svf and the parenthesis) command. An example of a descriptive filename is 15N13C_SF1DBD+SBS_cconhtocsy_35C. The program will create a directory with an `.fid` suffix and in this directory you will find four files: `fid`: which contains the NMR data, `text`: any title given for the sample/experiment using the `textvi` command before data acquisition was initiated, `log`: start and stop acquisition times and any error messages generated during the experiment, and most important of all `procpar`: which contains all the acquisition parameters.

Transferring NMR Data from the Inova to Abragam

1. Create a folder (using the `mkdir` command) in an appropriate directory below the `felix/data` directory. Have a separate folder for each project. For Felix, the filenames need to be succinct and should all be in lower case. Here is a guide. Let's consider npsnnohs.fid (data for a PAH2-SID complex). The first letter identifies the sample – in this case ^{15}N-labeled. For binary complexes, the second and third letters identify the two components with the component that is labeled given precedence. Subsequent letters identify the experiment: here nnohs is ^{15}N-edited NOESY-HSQC. Ideas for short names for CBCACONH (baon) and HNCACB (nab).
2. Go to the directory you just created and type `sftp ishwar@inova`.
3. Navigate to the directory where you saved your data on Inova. You actually have to go into directory with the `.fid` suffix (where the four files `fid`, `text`, `log` and `procpar` have been saved).
4. Confirm that the directory contains these four files by typing the `ls` command.
5. Type the command `mget *` and wait for your data to copy from Inova to Abragam.
6. When transfer is complete (i.e. all four files have been copied), type `exit` to return to the command prompt. Type `ls` again to check whether all four files were copied into the directory.

Processing NMR Data using Felix

1. Copy an appropriate Felix macro from Ishwar's `felix980/macs` directory to your `felix/macs` directory. Give it the same name as the data folder except ending with a `.mac` suffix. Edit the macro using the `vi` or `jot` editor.
2. Key items to change in any given macro include: names of the data file and matrix (again give it the same name as the data folder but with a `.mat` suffix). Be sure the matrix is saved in an appropriate project subdirectory under the

`felix/matrix` directory (this is defined by `matpfx` in the macro). Set `numd2` and `numd3` to `2*ni` and `2*ni2`, respectively, from the `procpar` file. Make sure appropriate window functions, zero-filling and data reduction are being applied and the matrix size is appropriate by scrolling through the macro. Save the macro.

3. Always launch Felix from your Felix startup directory (`felix`) and execute the macro from the command line. Be sure to perform any phase correction if the peaks are not purely absorptive (have strong positive and negative components in any of the dimensions). Apply baseline corrections if you see horizontal stripes of the same sign in the processed spectrum.