**Processing $^{15}N/^{1}H$ ZZ exchange datasets and extracting peak intensities for time series analysis**

We typically run $^{15}N/^{1}H$ ZZ exchange datasets as an interleaved series of 2D spectra (each with an individual ZZ delay) to minimize the impact of potential sample degradation or aggregation on the time series data. In this case, the 15N_scotch_v2 pulse sequence is set up to array dso, phase.

1. Grab data from Plumeria and gzip fid file as usual.
2. Edit processZZ.com macro; check parameters with varian command as usual, then update as below:

```
#!/bin/csh

gzcat ./fid.gz | var2pipe -noaswap \
  -xN              1024  -zN               128  \  -yN             5\
  -xT               512  -zT                64  \  -yT             5\
  -xMODE        Complex  -zMODE        Complex  \  -yMODE   Real\
  -xSW          8000.00  -zSW         1519.988  \  \
  -xOBS         599.749  -zOBS          60.779  \  \
  -xCAR           4.667  -zCAR         120.143  \  \
  -xLAB              H1  -zLAB             N15  \  -yLAB      dso\
  -ndim               3  -aq2D           States  \
| nmrPipe  -fn POLY -time                                          \
| nmrPipe  -fn SP -off 0.35 -end 0.95 -pow 2 -c 0.5                \
| nmrPipe  -fn ZF -zf 1 -auto                                      \
| nmrPipe  -fn FT -verb                                            \
| nmrPipe  -fn PS -p0 99.0 -p1 0.0 -di                             \
| nmrPipe  -fn ZTP                                                 \
| nmrPipe  -fn LP -fb                                              \
| nmrPipe  -fn SP -off 0.35 -end 0.98 -pow 2 -c 0.5                \
| nmrPipe  -fn ZF -zf 1 -auto                                      \
| nmrPipe  -fn FT -verb                                            \
| nmrPipe  -fn PS -p0 0.0 -p1 0.0 -di                              \
| nmrPipe  -fn ZTP                                                 \
| nmrPipe  -fn TP                                                  \
| nmrPipe  -fn ZTP                                                 \
| nmrPipe  -fn TP                                                  \
| nmrPipe  -fn POLY -auto                                          \
| nmrPipe  -fn EXT -x1 11ppm -xn 6.2ppm -sw                       \
| pipe2xyz -out FTs/CP165a_%02d.ft -ov -verb
```

This should reflect the number of 2D spectra you collected at various dso values -- nmrPipe will process all 2D spectra together, then split out an ft for each fid to look at in nmrDraw

The interleaved spectra are split according to the dso (ZZ delay)

This will extract just the region from 11 ppm to 6.2 ppm to show in nmrDraw.

Processed ft files will be saved in a new directory named FTs as a series based on the experiment number (CP165a in this case), followed by an underscore and iterating a number for each ft in order as run (i.e. CP165a_01.ft, CP165a_02.ft, etc).

3. Save macro, process and open in nmrDraw. Double click on FTs in bottom window to open new directory containing processed data. Double click on top ft file (CP165a_01.ft), then edit file name after the under-score to replace the number is %02d.ft. This will simultaneously open all ft files as a series of 2Ds -- you can 'step' through the different spectra with the Z button (upper left). Phase the first spectrum (typically with dso set to zero). Get P0 value, correct processing macro and re-process.
4. Once you're happy with the data processing, go to FTs file and convert ft files to nv format using the command:

% pipe2xyz -in CP165a_01.ft -nv -out ppih1.nv

[repeat as needed to convert all files]

5. Write a time file in nedit. Indicate nv file number on the left, single space, delay time (in any units):

ppihtime.txt – /Users/roma/data/CP167/nv/

File Edit Search Preferences Shell Macro Windows He

```
1 0
2 0.25
3 0.5
4 0.75
5 1
6 1.25
7 1.5
8 1.75
9 2
10 2.5
11 3
```

Save time file as a .txt file in Unix format.