

Processing ¹⁵N/¹H ZZ exchange datasets and extracting peak intensities for time series analysis

We typically run ¹⁵N/¹H 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).

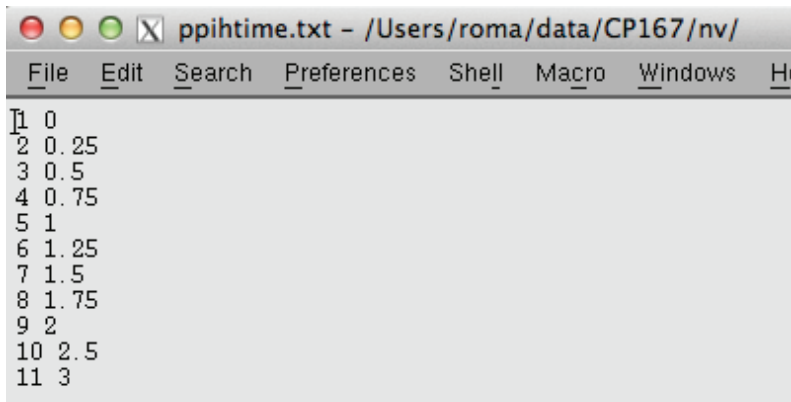
3. Save macro, process and open in nmrDraw. Double click on FTs in bottom window to open new directory containing processed data. Double click on top ft file (CP165a_01.ft), then edit file name after the underscore to replace the number is %02d.ft. This will simultaneously open all ft files as a series 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):



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