Zero Filling in 2D

NMR SPECTROSCOPY

(Xwinnmr on PC, version 3.5)

on

DPX 200, DPX 300, and DRX 500

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Log in and start xwinnmr.

1.   Select a 2D dataset with **search**, for instance a COSY spectrum.

2.   If you do not own the dataset, make a copy for yourself with the **wrd** command.
      Type **wrd↵** this is the command for copying the dataset which is on screen to another disk
      (home or other place) for permanent storage and at the same time **change the ownership** of
      the files.

      Enter target data set **NAME:**   **EXPERIMENTNAME↵**   (use your own
                                              expname)
      Enter target data set **EXPNO:**   **1↵** (use the expno seen in the top part of the xwinnmr
                                              window).
      Enter target data set **PROCNO:**   **1↵** (use the procno seen in the top part of the xwinnmr
                                              window).
      Enter target disk unit **DU:**   **M:↵** (the dataset will go to your home directory on
                                              another computer for permanent storage, use **D:** if you
                                              don't need a permanent copy).
      Enter target user name **USER:**   **uio user name↵**   (your own uio user name).

3.   Use **search** again to find the dataset which now is owned by you, then **append** and **apply** it
      to the xwinnmr window and **xfb** to Fourier transform it in both directions. You can not work
      properly with a dataset not owned by your self.   If the computer you are using does have another plotter
      attached than the one used under acquisition use **edo** (edit output) to select the new plotter. The data set does regretfully
      remember the plotter name connected to the computer used to acquire the spectrum.

4.   Scale the spectrum on the screen with appropriate buttons on the left part of the xwinnmr
      window, ***2** or **/2**. Observe that the peaks in the spectrum most probably are "longer" in one
      dimension (F1, υ1, ω1, t1 axis) than the other axis (F2, υ2, ω2, t2). The resolution is better
      in the observed dimension (F2) than the dimension originating from the variable delay (F1)
      inside the pulse sequence.

5.   Type **eda** to see acquisition parameters. Look for the parameter **TD** in the F2 dimension -
      this number if often 1024. Look then for the **TD** number in the F1 dimension. This
      parameter is often 128. The lower number in the F1 dimension relative to the F2 dimension
      is the reason for the elongated peaks in the F1 dimension. Increasing the TD in F1
      dimension drastically increases the experiment time. Eda parameters can only be changed
      before the experiments starts.

6.   Type **edp** to see processing parameters. Look for the parameter **SI** (size) in both F1 and F2 dimension.(size). **edp parameters can be changed after the experiment is finished.** This is the basis for manipulating the data and making the spectrum look better by ZERO FILLING. With SI (F2) 512 and SI (F1) 64 no zero filling is performed. Zero filling in the F2 dimension has little effect on the appearance of the spectrum. Zero filling once or twice does not harm though. SI (F2) at 1024 and SI (F1) at 128 one zero filling is performed in both dimensions. With SI (F2) at 1024 and SI (F1) at 256 one zero filling is performed in the F2 dimension and a double zero filling is performed in the other dimension. **<u>Try out different combinations to see how the spectrum changes.</u>** Use increasing numbers in **procno** (set in edc) for each processing. Plot all the different spectra.

7.   If you are confused with the fact that SI=TD/2 when no zero filling is performed please remember that the FID of a 1D spectrum has the double number of points compared to the real part of a 1D spectrum.

8.   Try also to change WDW between SINE, QSINE, EM and GM. WDW is the so called window function which will give different parts of the FIDs different importance. A separate manual for WDW will come out shortly.