Getting VNMR Plots into Publishable Form

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I. Using Native VNMR Plotting

- See other notes on VNMR plotting online to get the plot into an acceptable form when printing out on the facility printers.

- Change the plotter using the **nextplotter** command until it is performing postscript printing; on some Sun workstations, this is the plotter **postfile** but on others it will be **Shadow_plot** or **gkar_plot** (or similar).

- Instead of using the command **page** use:

  page('*filename*')

  This command will produce a postscript file in your current directory (which you can see with the vnmr command **pwd .**

- The vnmr macro **plot2dhr** is useful for giving nice plots of 2D spectra. **plot2dhr** automatically finishes with the **page** command. **plot2dps** is identical, but with the **page** command removed. Once you get a plot you like with **plot2dhr** off the printer, use **plot2dps** with identical options, then use a **page('*filename*')** command, and use the resulting postscript file *filename* as described in the next paragraph.

- The postscript file *filename* can be transferred (using ftp) and imported into any good quality graphics editing program for addition of annotations, fixing of axis tics and fonts, thickening of spectra lines, addition of colors, etc. Facility staff use CorelDraw (cgf) and Illustrator (mi), and can answer some (limited) questions on this subject. For example, use of the suffix .prn on the filename is helpful when using CorelDraw.

II. Getting VNMR data into NUTS

NUTS works fine for 1D data, but cgf prefers vnmr for producing figures from 2D data. Other programs, such as SPARKY, are likely better than NUTS for 2D data.

A.. Extracting 1D spectra arrayed data sets, for importation into NUTS:

1. Suppose the array dataset is in exp1. Then do the following to extract the 8th fid:

   jexp1 df(8) clradd add

This set of commands will copy the 8th fid and all the parameters into exp5 (which is used automatically by the **clradd** command; **clradd** will delete whatever was in exp5, so make sure to save anything important there before proceeding). Then:

jexp5 wft [phase the data] svf('*anyname*')

transforms the 8th spectrum, let's you phase is, and writes a "normal" VNMR file.

2. If the arrayed parameter is important (suppose it is a variable temperature dataset), it is easiest to add the parameter value into a label like text. But if you really want the parameter in the dataset changed, then use the following commands in order:

jexp5 temp=21.5 arraydim=1
groupcopy('current','processed','acquisition')
svf('*anyname*')

The 2nd command updates the acquisition parameters from the (temporary) current parameters before you resave the fid.

Another common variable would be time (from the start of acquisition). Here the advise is to add this variable to the text label prior to saving the data, e.g.:

atext('time from start of acquisition = 103 s')

and/or to add the information to the name of the new fid folder, e.g.:

svf('sample_q103_spec5_tstart_103s')

B.. Getting NUTS spectra into graphics programs for clean-up and annotation, etc.:

1. The simplest ways of porting NUTS spectra to graphics programs do not provide the best quality (e.g., go to 500% in Word, and you will see a bit of pixelation), they are sufficient for most publication/supplemental information purposes. You can do better via a variety of methods; ask if this is required (and see some notes below).

The simple method is to use the menu commands:

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inside of NUTS. Then use a normal paste into Word. One has to change the frame of the pasted figure inside Word to get text boxes and ChemDraw structures overlaying the spectra. It should be easy to figure out how to get the colors changed, or go to simple black and white.

2. A (much) better method is to use

   EDIT → COPY PRINTER DC ENHANCED METAFILE TO CLIPBOARD

   in a true graphics program like CorelDraw or Illustrator. Some playing with what printer is being used on your particular PC/Mac may be necessary. Please do *not* ask for assistance with this from facility staff; we simply do not have time to contend with these kinds of questions (i.e., you're on your own). See the online NUTS documentation at

   www.acornnmr.com

   for more information and some examples.