Common Plotting Commands and Parameters in VNMR

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I. Common 1D Plotting Commands

- see figures at end of this document for graphical description of main parameters used for plotting
- display the axis using **dscale(0)** and **axis='p'**, or use the macro **dsx**
- plot spectra using the following commands:

pl ; plots spectrum with **sc** being cm in from *right* side **wc** being width in cm

pap ; plots all parameters along left hand side, or **ppa** for the major parameters only; does plot out **text**, which can be entered manually, but easiest way is to use the CDE File Manager to go to ~/vnmrsys/exp1 (assuming working in exp1) and double click on **text** file; simple editing of the file can then be performed

ppf ; plots peak pick
th controls threshold height used);
dpf will show peak picks on screen
dll lists peak picks with intensities (**printon dll printoff** will print)

pirn ; prints integral values under axis:
– start with **cz** to clear integrals
– click MAIN MENU DISPLAY INTERACTIVE PARTIAL INTEGRAL
– type **region** (if you don't like the regions, start again with **cz** and use the RESETS button to enter regions with the mouse manually)
– type **intnorm** or use UWMACRO MORE NORMINT or DISPLAY NORMINT [**adjism** is Varian's not-so-good command] to adjust the peak amplitude
– enter **vp=12** to get axis out of list area
– integrals will plot with **pl** when on screen; **pirn** is needed to list values below axis

II. Notes for Inset Plots

1. Get the 1D full spectrum plot looking as you want it plotted, then:

   axis='p' pl pscale ↵ ;this plots the full spectrum and axis in ppm

   s2 ↵ ;this important command saves the display region

2. Place the two cursors about the region to be inset

inset then move and expand with left and right mouse buttons

[note that the full spectrum is ***not*** really present; vnmr simply did not erase it from the display, so you can better see where to place the inset]

axis='h' pl pscale ↵ ;this plots the inset with axis in Hertz

page ↵ ;tells the plotter you are finished and ejects page from printer

3. **r2** ↵ ;recalls the saved display region 2, returning normal display

E. Phase-Sensitive 2d Data Workup and Plotting

- often should not need to phase DQCOSY data at all
- ***phase sensitive*** data should be processed something like the following:

  – set **pmode='full'** ; allows phasing along F2 in 2d spectrum

  – **wft(1)** ; transform just first spectrum

  – **wtia** ; interactive phasing; middle button scales, left sets **lb**

  – **wft1da** ; perform first transform (on t_2 dimension)

  – if integrals have been setup (best on high-res 1d done prior to setting up dqcosy), then **bc('f2')** can sometimes work wonders here

  – click on **TRACE** and select strong intensity trace
  ; trace='f1' changes columns → rows, trace='f2' goes back

  – **wtia** ; interactive phasing on t_1 trace, left button sets **lb**/**gf**

  – **wft2da** ; performs second (or both) transform(s)

  – pick off two (or three) traces that have crosspeaks
  ; downfield trace save number as **r1**
  ; upfield trace save number as **r2**

  – **ds(r1)** do 0-order phase only

  – **ds(r2)** do 1st-order phase only (click left mouse button on downfield position sets toggle pt)

  – iterate between **ds(r1)** and **ds(r2)** to get good phase

  – **dconi** ; should now have good phasing

  → **trace='f2' dconi** allows phasing along F2 (similar to above) if needed

  – if integrals have been setup (as above), and only if **fn1=fn**, then **bc('f1')** can sometimes work wonders here

  – to plot, **plot2dhr** is a new macro that works quite well; if you want 1d projections, load the high-resolution 1d into a separate experiment before issuing the macro

command. Otherwise, I like parameters: **wc=130 wc2=wc sc=0** ; this leaves room for a vertical projection or to print parameters on the page (use **disp2d** to set these)

- maximum printable parameters on 8.5×11 paper are **wc=230 wc2=150**
- **rl(..p)** gives F2 referencing, **rl1(..p)** gives F1 reference
- use **plot2dhr** (preferred) or **pconpos** or **pconneg** to plot phase sensitive spectra