Some Useful Commands and Parameters for Plotting a 1D Spectrum

- **ppa**: `page => last command issued`
- **pl**: `plot the spectrum`
- **pscale**: `p p m`
- **wp**: `Sample directory: indanone_carlos_18Sep2000`
- **sp**: `file: PROTON, Mercury-300BB “nmr500v.princeton.edu”`

Indanone in CDCl₃
H¹ spectrum at RT
300 MHz

Archive directory: /export/home/vnmrl/vnmrsys/data
Sample directory: indanone_carlos_18Sep2000
Pulse Sequence: s2pul
Solvent: CDCl₃
Ambient temperature
File: PROTON
Mercury-300BB “nmr500v.princeton.edu”

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.983 sec
Width 2403.8 Hz
8 repetitions
OBSERVE: H¹, 300.0559606 MHz
DATA PROCESSING
Gauss window 0.555 sec
Center at 0.224 sec
FT size 131072
Total time 0 min, 24 sec
... Plotting a 1D Spectrum (cont.)

- `indanone in cdc13`
- `H1 spectrum at RT`
- `300 MHz`

Archive directory: /export/home/vnmrl/vnmrsys/data
Sample directory: indanone_carlos_18Sep2000
Pulse Sequence: s2pul

```
dpir => to display integrals; pir => to plot integrals
```

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- `th <= value>` or
- `adjust the vertical position of the horizontal yellow line by pointing the cursor to it, hold the left button of the mouse, and drag it up or down`
Plotting a 1D Spectrum (cont.)

indanone in cdc13
H1 spectrum at RT
300 MHz

Archive directory: /export/home/vnmrl/nmrsys/data
Sample directory: indanone_carlos_18Sep2000
Pulse Sequence: s2pul

Interactive → Set Int → Value? 3

cursor
inset
Some Useful Commands and Parameters for Plotting a 2D Spectrum

➢ To display contour levels (color display) interactively:
  • dconi
    ✓ adjust the 2D threshold by clicking on the buttons vs+20% and vs-20%

➢ To plot contour levels:
  • pcon(number of levels, spacing between levels)
    ✓ Example: pcon (20,1.2)
  • dpcon(number of levels, spacing between levels)
    - display contour plot on screen

➢ To plot a grid:
  • plgrid (start of grid in F1, spacing in F1, start of grid in F2, spacing in F2, )
    ✓ Example: plgrid (1p,0.5p,1p,2p)
  • grid – display grid on screen

➢ Parameters:
  • sc, wc - start of chart in F1, width of chart in F1
    ✓ Example: sc=0 wc=110
    • Obs – units in mm
  • sc2, wc2 – start of chart in F2, width of chart in F2
    ✓ Example: sc2=0 wc2=110
    • Obs – units in mm
  • sp, wp – start of plot in F2, width of plot in F2
    ✓ Example: sp=-0.5p wp=11p
  • sp1, wp1 – start of plot in F1, width of plot in F1
    ✓ Example: sp1=-0.5p wp1=11p
... for Plotting a 2D Spectrum (cont)

Gra m icidin-S
m DMSO
10/11/2000

Sample directory: gramicidin_11Oct2000

Pulse Sequence: gCOSY

Solvent: DMSO
Temp. 25.0 C / 298.1 K

File: gCOSY

Mercury-300BB "nmr500v.princeton.edu"

Relax. delay 1.000 sec
Acq. time 0.171 sec

Width 3000.3 Hz
2D Width 3000.3 Hz

4 repetitions
256 increments

OBSERVE H1, 300.0573859 MHz

DATA PROCESSING

Sinc. bell 0.089 sec
Shifted by 0.008 sec

F1 DATA PROCESSING

Sinc. bell 0.041 sec

F1 size 2048 x 2048

Total time 22 min, 39 sec

1D high resolution spectrum

ppa
Two-Dimensional NMR

Example: Gramicidin-S

COSY

TOCSY