

# Some Useful Commands and Parameters for Plotting a 1D Spectrum



*page => last command issued*

indanone in cdcl3  
H1 spectrum at RT  
300 MHz

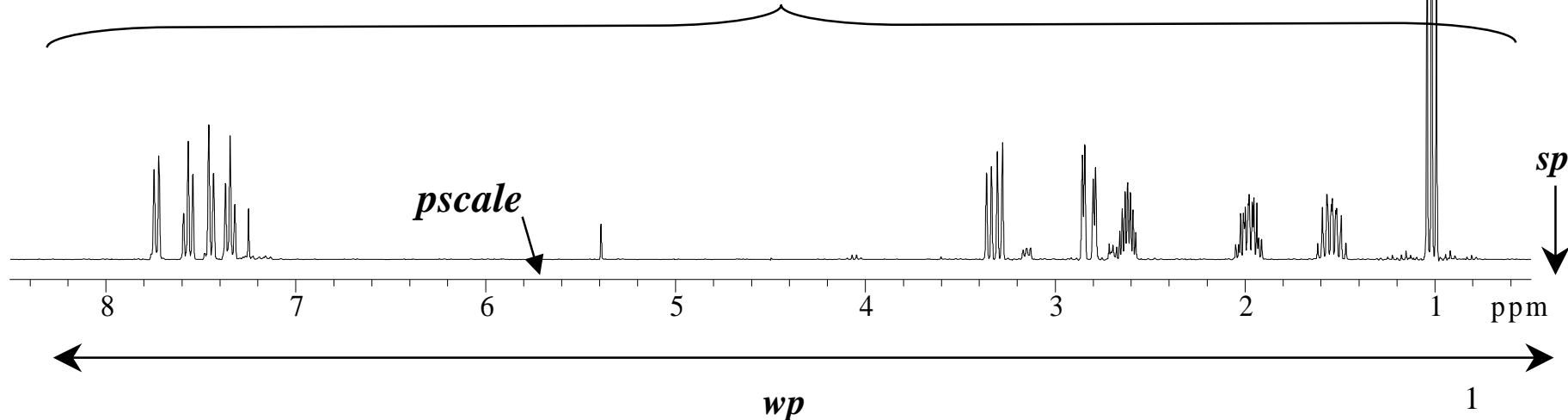
Archive directory: /export/home/vnmr1/vnmr sys/data  
Sample directory: indanone\_carlos\_18Sep2000

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

*ppa*

*pl => plot the spectrum*



## ... Plotting a 1D Spectrum (cont.)



*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

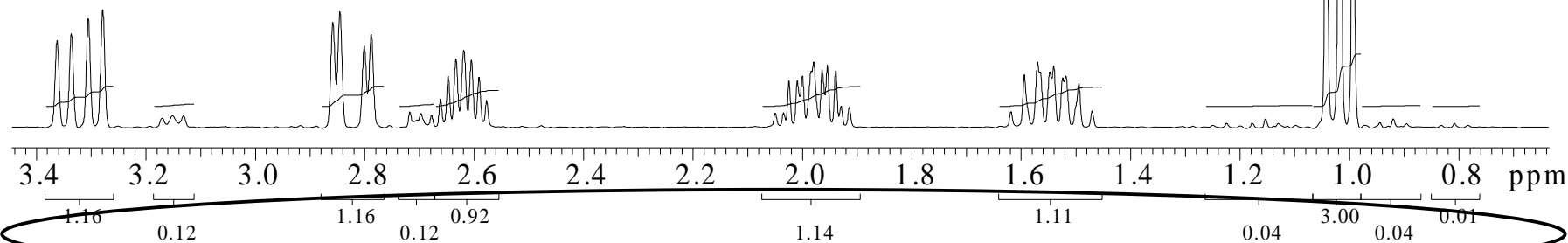
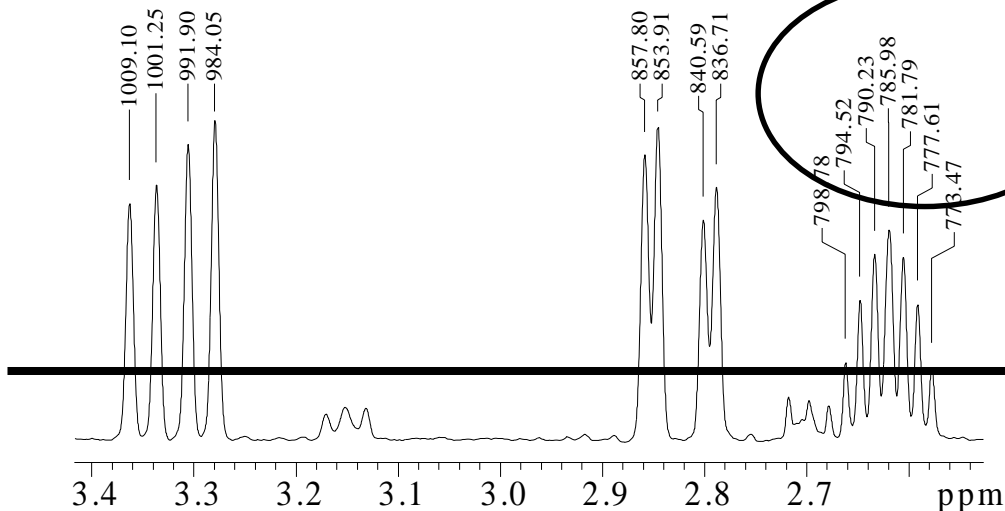
indanone in cdcl3  
H1 spectrum at RT  
300 MHz

*pltext*

Archive directory: /export/home/vnmr1/vnmr5s/data  
Sample directory: indanone\_carlos\_18Sep2000

Pulse Sequence: s2pul

*axis='h'* ppf



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

## ... Plotting a 1D Spectrum (cont.)

Interactive



Set Int

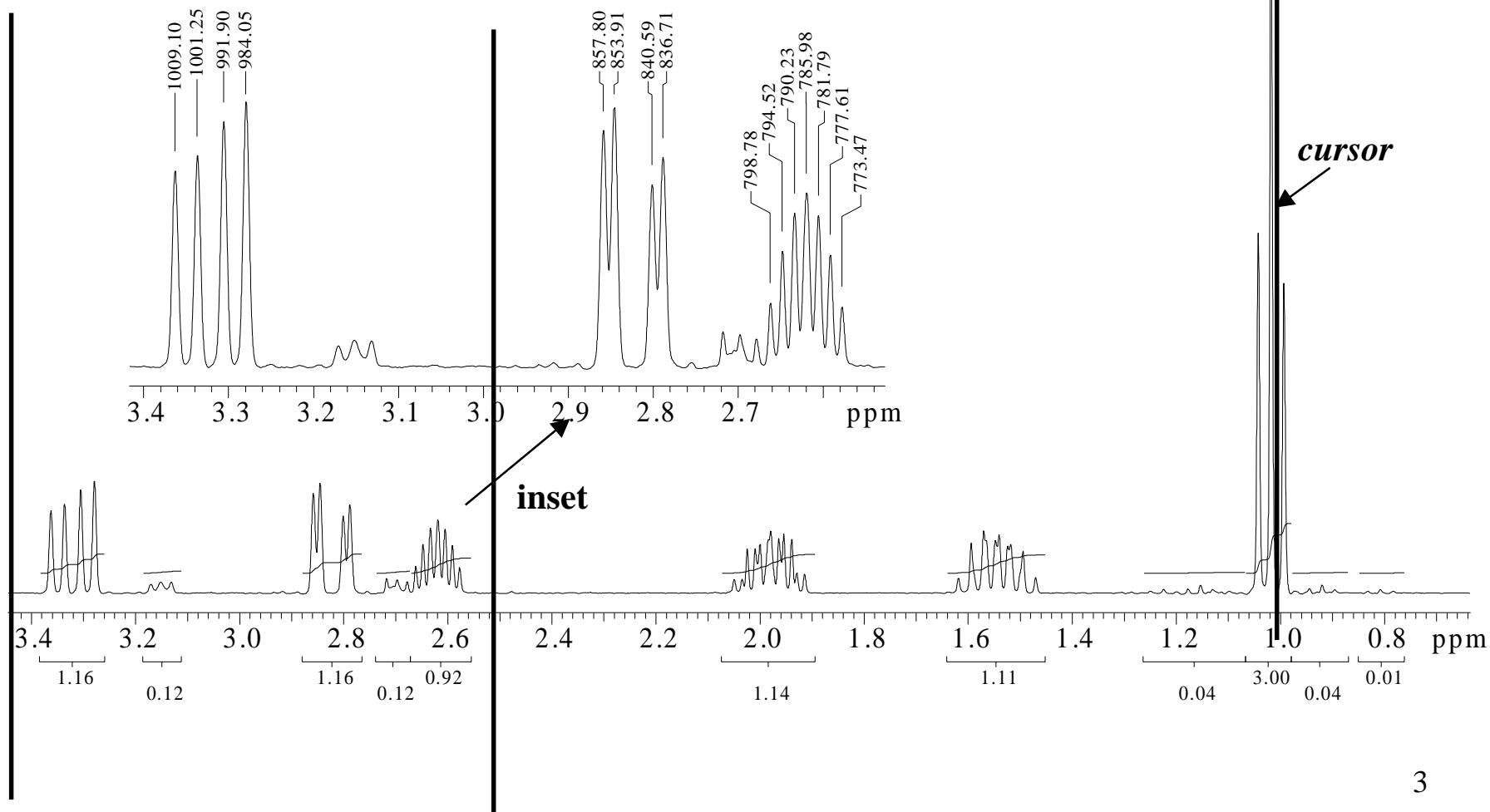


Value? 3

indanone in cdc13  
H1 spectrum at RT  
300 MHz

Archive directory: /export/home/vnmr1/vnmrSYS/data  
Sample directory: indanone\_carlos\_18Sep2000

Pulse Sequence: s2pul



# Some Useful Commands and Parameters for Plotting a 2D Spectrum



## ➤ To display contour levels (color display) interactively:

- **dcon**
  - ✓ adjust the 2D threshold by clicking on the buttons **vs+20%** and **vs-20%**

## ➤ To plot contour levels:

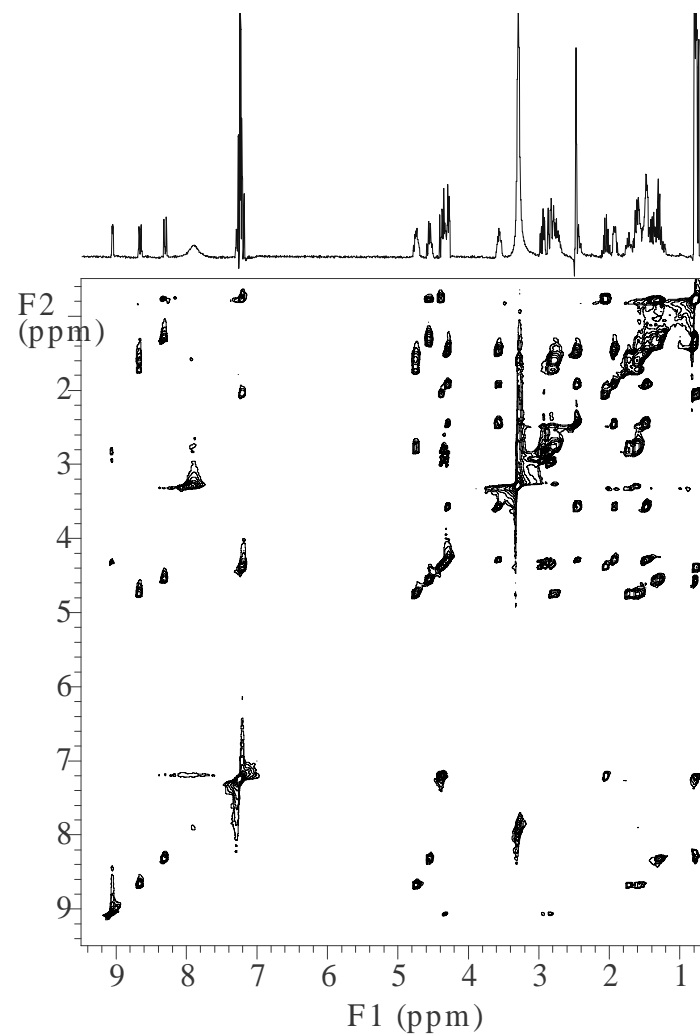
- **pcon**(number of levels, spacing between levels)
  - ✓ Example: **pcon (20,1.2)**
- **dpcon**(number of levels, spacing between levels)
  - display contour plot on screen

## ➤ 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)



1D high resolution spectrum

**ppa**

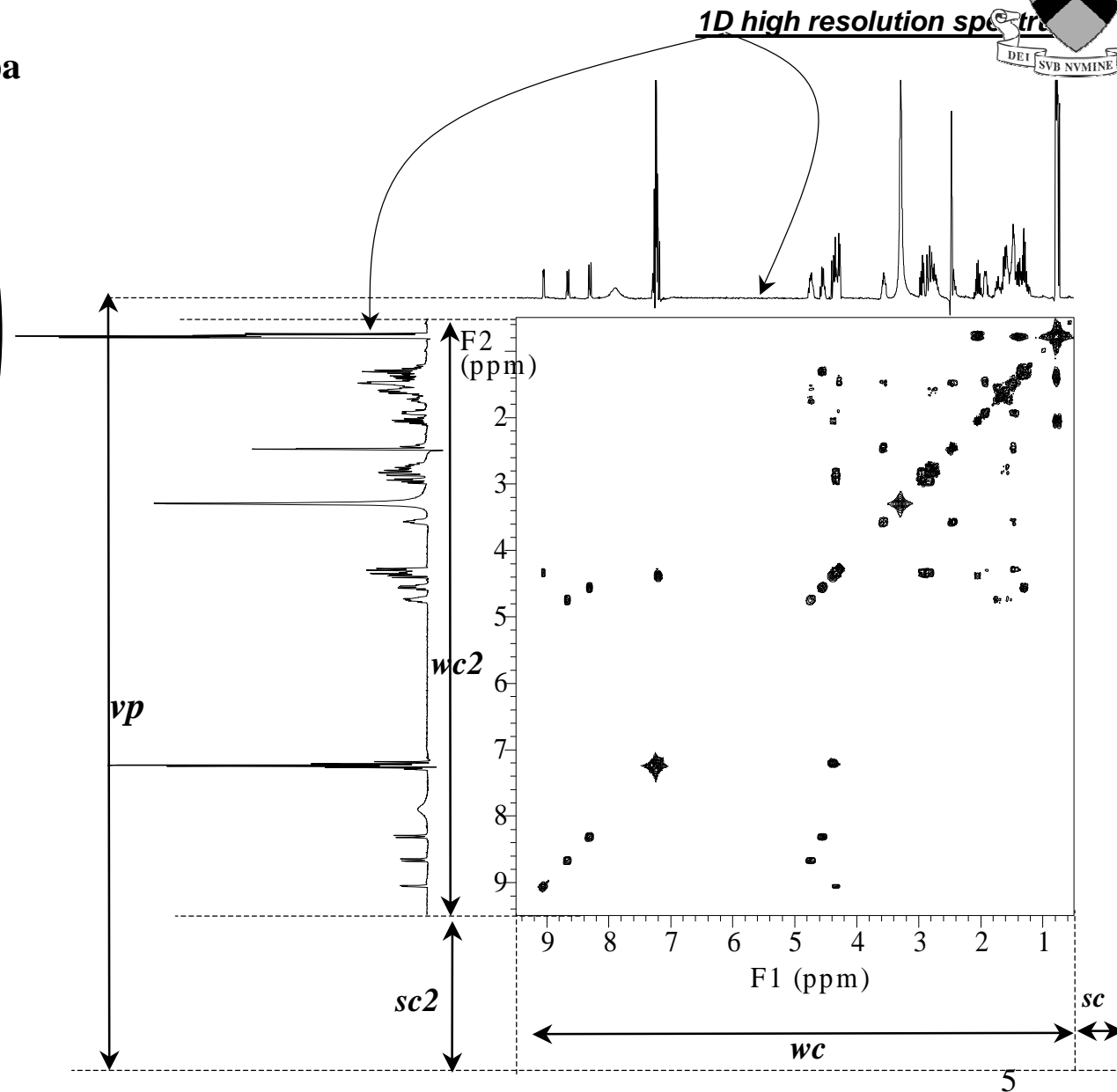
Gramicidin-S  
in DMSO  
10/11/2000  
gCOSY

Sample directory: gramicidin\_11Oct2000

Pulse Sequence: gCOSY

Solvent: DMSO  
Temp. 25.0 C / 298.1 K  
File: gCOSY  
Mercury-300BB "nmr500v.princeton.edu"

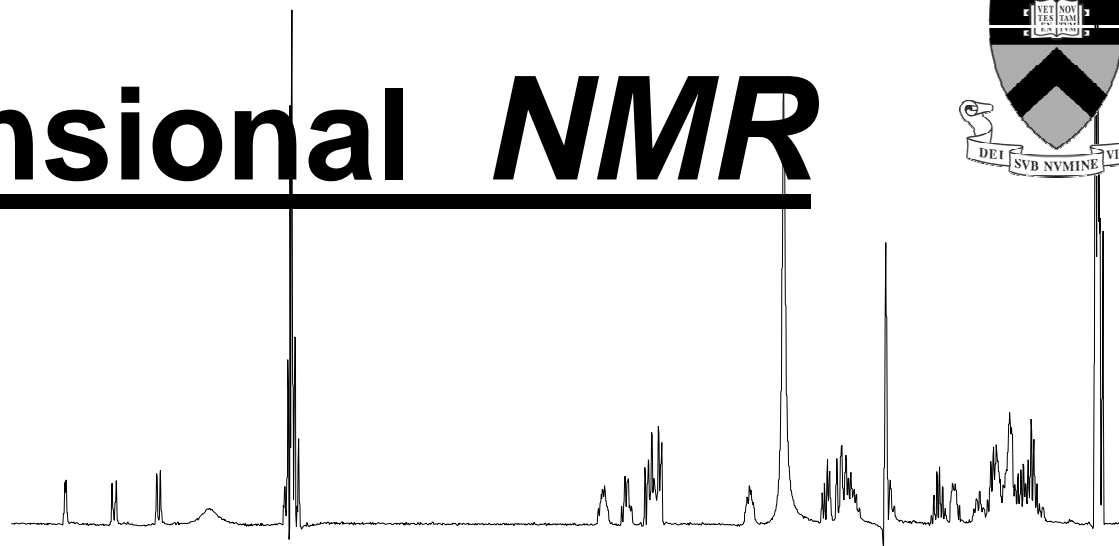
Relax. delay 1.000 sec  
Acq. time 0.171 sec  
Width 3000.3 Hz  
2D Width 3000.3 Hz  
4 repetitions  
256 increments  
OBSERVE H1, 300.0573859 MHz  
DATA PROCESSING  
Sine bell 0.089 sec  
Shifted by 0.008 sec  
F1 DATA PROCESSING  
Sine bell 0.041 sec  
FT size 2048 x 2048  
Total time 22 min, 59 sec



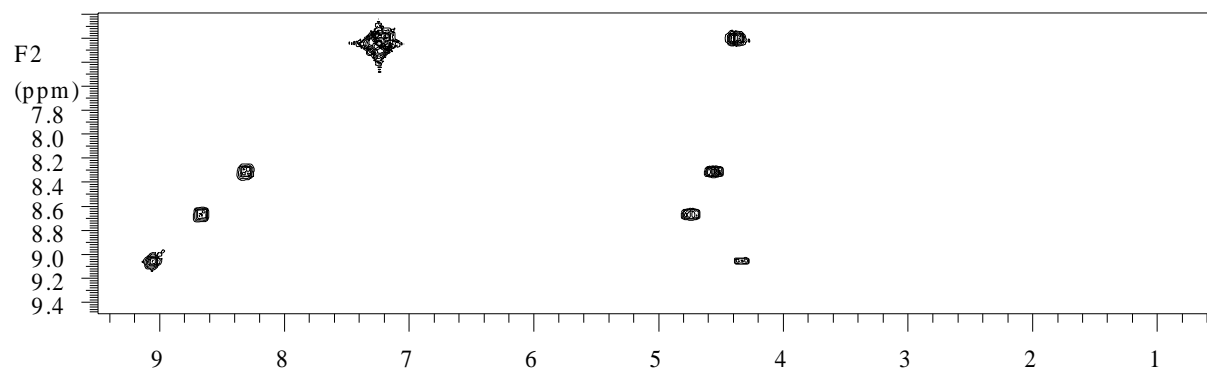
# Two-Dimensional NMR



*Example: Gramicidin-S*



**COSY**



**TOCSY**

